



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:28 AM UTC

PDB ID : 1L5R / pdb_00001l5r
Title : Human liver glycogen phosphorylase a complexed with riboflavin, 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.; Myszkka, 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

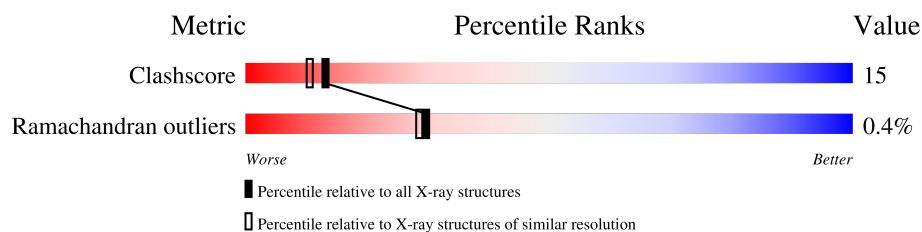
1 Overall quality at a glance

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)

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	 63% 28% • 7%
1	B	847	 63% 28% • 7%

2 Entry composition [i](#)

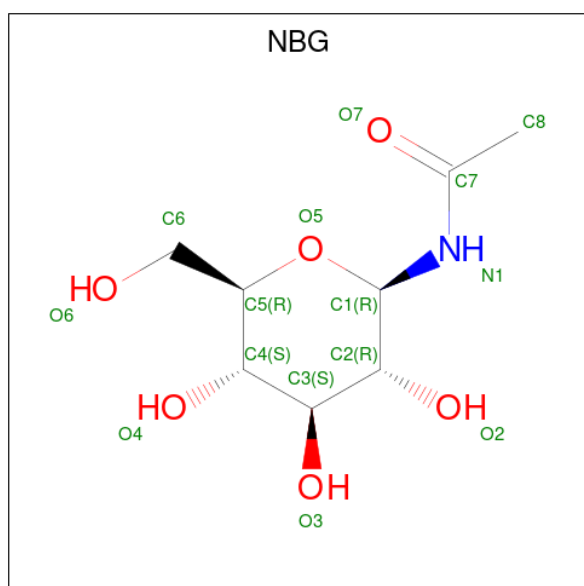
There are 7 unique types of molecules in this entry. The entry contains 13497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	790	Total	C	N	O	S	0	0	0
			6417	4125	1089	1174	29			
1	B	791	Total	C	N	O	S	0	0	0
			6423	4128	1090	1176	29			

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



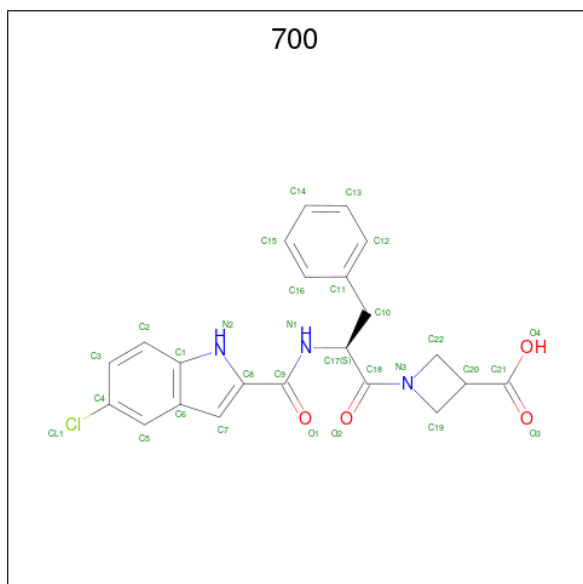
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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



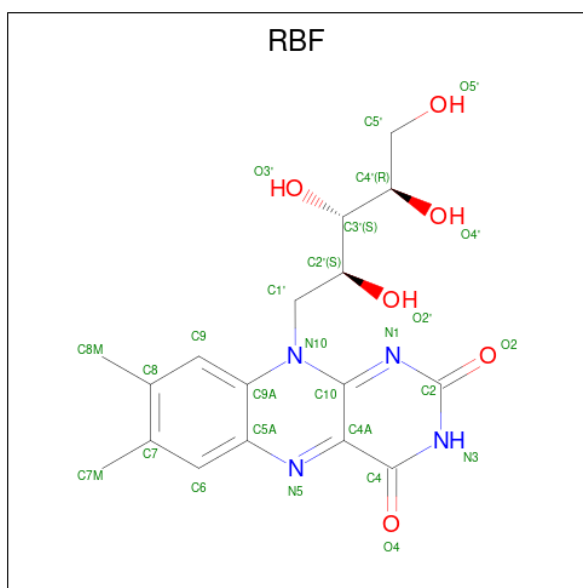
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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



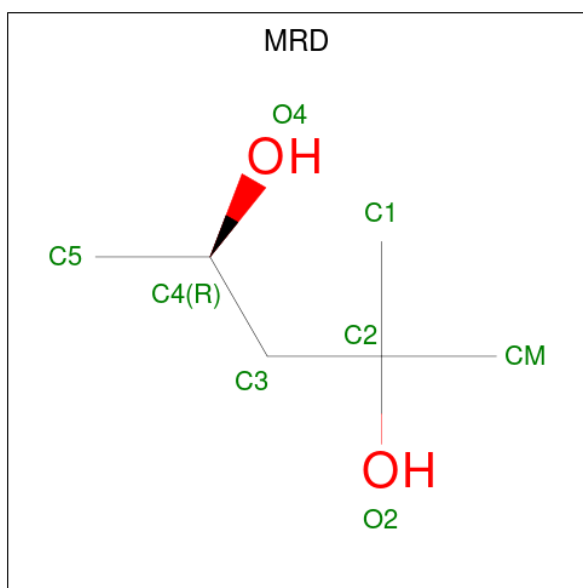
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is RIBOFLAVIN (CCD ID: RBF) (formula: $C_{17}H_{20}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			27	17	4	6		

- 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	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	307	Total 307	O 307	0	0
7	B	240	Total 240	O 240	0	0

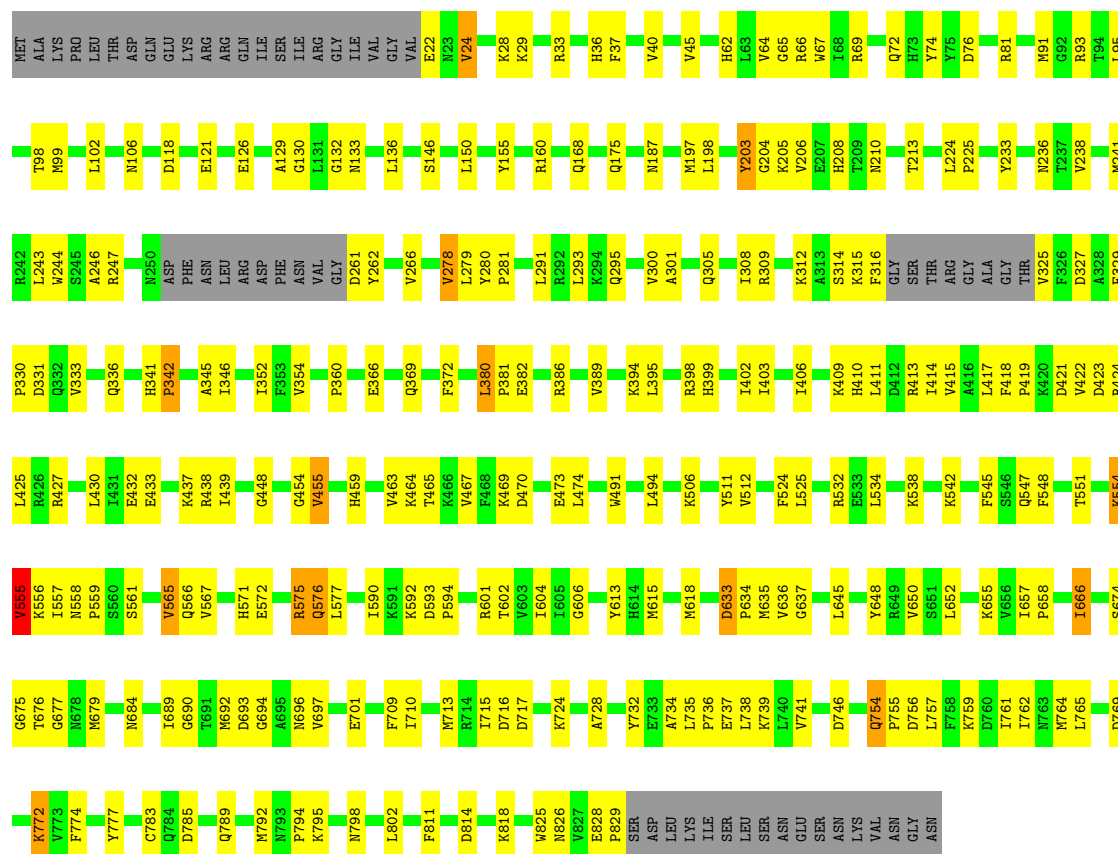
3 Residue-property plots

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: 



I761	I666	K554	L430	THR	Y233	M99
I762	I763	K555	I431	V325	N236	L102
M764	S674	K556	E432	F329	T237	N106
L765	M675	I557	E433	P330	V238	E110
D769	T676	N558		D331		Y113
K772	M677	S561	K437	Q332	L243	D118
M773	M679	S562	R438	V333	W244	E121
F774	N684	V665	I439	Q336	S245	E126
		Q566	C445		A246	A129
		V667			R247	N133
	I689	H571	G448	H341	N250	G135
C783	G690	E572		P342	ASP	L136
M692	T691	E573	G454	A345	PHE	S146
D785	M693	D693	V455	I346	ASN	L150
K786	G694	R575	H459	I352	LEU	E155
	A695	Q576		F353	ARG	R160
Q789	N696	L577	V463	F354	ASP	Q168
M792	V697	K592	K464	V354	PHE	K169
M793	E701	D593	E473	R386	ASN	L170
F794	L708	P594	L474	V389	VAL	L171
K795	F709	V599	V467	F372	GLY	Q175
L802	I710	P600	D470	A373	D261	E179
		R601		Y374	Y262	Q182
		T602	E473	E382	V266	S192
D814	M713	T603	L474	R386	E273	M197
K818	R714	I604		V389		L198
W825	L715	I605	L487	K394	V278	Y203
N826	D716	G606	P488		L279	C204
E828	D717	G606			Y280	V206
	K724	Y613	W491	H399	P281	H208
P829		H614	L494	L400	N282	T213
S830	A728	M615		E401	D283	I216
		M618	K506	I402	N284	L224
ASP	Y732	D633	V512	I403	F285	P225
LEU	E733	P634	K513	I406	V300	C225
LYS	L734	M635		A409	A301	
ILE	L735	G636	F524	H410	Q305	S192
SER	P736	V637	L525	L411		
SER	E737	G637		H412	I308	M197
SER	K739		D528	R413	R309	L198
ASN	L740	L645	R532	R413	I414	
GLU	V741	E646		W415	R310	Y203
SER		F648		A416	F311	C204
ASN		V649	K538	L417	K312	K205
VAL	D746	V650		F418	A313	V206
GLN	P752	S651	K542	P419	E207	E207
ASN	K753	L652	L543	A420	K315	H208
GLY	F754		K544	K420	F316	
ASN	P755	K655	F545	D421	GLY	T213
	T756	V656	S546	V422	THR	
	L757	I657	Q547	D423	SER	I216
	F758	P658	F548	R424	ARG	L224
	K759	A659		L425	GLY	P225
	P760	T660	T551	R426	ALA	C225

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	124.42Å 124.42Å 124.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.61 – 2.10	Depositor
% Data completeness (in resolution range)	95.5 (55.61-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13497	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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, RBF, MRD

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	0.53	0/6561	1.01	44/8873 (0.5%)
1	B	0.50	0/6567	1.00	40/8881 (0.5%)
All	All	0.51	0/13128	1.00	84/17754 (0.5%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	VAL	N-CA-C	8.86	121.24	108.48
1	B	565	VAL	N-CA-C	8.65	120.58	108.12
1	B	575	ARG	N-CA-C	8.31	123.15	111.52
1	A	575	ARG	N-CA-C	8.20	122.71	111.39
1	A	64	VAL	N-CA-C	7.88	118.42	110.23
1	B	64	VAL	N-CA-C	7.40	118.13	110.36
1	B	576	GLN	N-CA-C	-7.35	104.19	113.01
1	B	354	VAL	N-CA-C	7.11	117.21	110.74
1	A	576	GLN	N-CA-C	-6.80	104.85	113.01
1	A	593	ASP	CA-C-N	6.79	126.30	119.24
1	A	593	ASP	C-N-CA	6.79	126.30	119.24
1	B	666	ILE	N-CA-C	6.69	123.25	109.34
1	A	91	MET	N-CA-C	6.68	121.18	112.89
1	B	593	ASP	CA-C-N	6.54	126.04	119.24
1	B	593	ASP	C-N-CA	6.54	126.04	119.24
1	A	676	THR	N-CA-C	-6.53	106.52	114.75
1	A	331	ASP	N-CA-C	-6.53	105.31	113.28
1	A	491	TRP	N-CA-C	6.34	120.03	112.93
1	B	129	ALA	N-CA-C	-6.33	95.29	107.57
1	A	666	ILE	N-CA-C	6.29	122.42	109.34
1	B	467	VAL	N-CA-C	6.28	116.45	110.42
1	B	262	TYR	N-CA-C	6.21	117.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	676	THR	N-CA-C	-6.21	106.93	114.75
1	B	331	ASP	N-CA-C	-6.14	105.79	113.28
1	B	633	ASP	CA-C-N	6.10	125.99	119.28
1	B	633	ASP	C-N-CA	6.10	125.99	119.28
1	B	91	MET	N-CA-C	6.07	120.41	112.89
1	B	772	LYS	N-CA-C	6.05	119.70	111.17
1	A	633	ASP	CA-C-N	6.03	125.92	119.28
1	A	633	ASP	C-N-CA	6.03	125.92	119.28
1	A	754	GLN	CA-C-N	6.03	127.38	119.84
1	A	754	GLN	C-N-CA	6.03	127.38	119.84
1	A	24	VAL	N-CA-C	6.01	116.75	110.62
1	A	278	VAL	N-CA-C	5.97	116.23	108.35
1	A	354	VAL	N-CA-C	5.95	116.16	110.74
1	B	754	GLN	CA-C-N	5.93	127.26	119.84
1	B	754	GLN	C-N-CA	5.93	127.26	119.84
1	B	455	VAL	N-CA-C	5.90	117.78	112.17
1	A	772	LYS	N-CA-C	5.90	119.49	111.17
1	B	491	TRP	N-CA-C	5.88	119.52	112.93
1	A	467	VAL	N-CA-C	5.87	116.06	110.42
1	B	278	VAL	N-CA-C	5.75	115.94	108.35
1	A	455	VAL	N-CA-C	5.75	117.63	112.17
1	A	37	PHE	N-CA-C	5.72	117.60	111.36
1	A	129	ALA	N-CA-C	-5.72	96.47	107.57
1	A	372	PHE	N-CA-C	5.70	119.38	110.32
1	B	37	PHE	N-CA-C	5.69	117.57	111.36
1	B	734	ALA	N-CA-C	5.66	117.53	111.36
1	B	372	PHE	N-CA-C	5.66	119.31	110.32
1	A	203	TYR	CB-CA-C	-5.58	110.15	116.63
1	B	280	TYR	CA-C-N	5.58	126.82	119.84
1	B	280	TYR	C-N-CA	5.58	126.82	119.84
1	B	602	THR	N-CA-C	-5.58	98.25	108.02
1	A	650	VAL	N-CA-C	5.56	116.20	110.36
1	A	380	LEU	CA-C-N	5.55	125.21	119.05
1	A	380	LEU	C-N-CA	5.55	125.21	119.05
1	A	811	PHE	N-CA-C	5.55	119.14	112.93
1	B	182	TRP	N-CA-C	5.54	119.14	112.38
1	A	333	VAL	N-CA-C	5.53	116.09	108.12
1	B	650	VAL	N-CA-C	5.53	116.17	110.36
1	B	203	TYR	CB-CA-C	-5.50	110.25	116.63
1	A	262	TYR	N-CA-C	5.49	116.94	111.07
1	A	280	TYR	CA-C-N	5.48	126.69	119.84
1	A	280	TYR	C-N-CA	5.48	126.69	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	684	ASN	N-CA-C	5.46	118.95	112.72
1	B	684	ASN	N-CA-C	5.44	118.92	112.72
1	B	333	VAL	N-CA-C	5.43	115.94	108.12
1	A	734	ALA	N-CA-C	5.42	117.19	111.28
1	B	216	ILE	N-CA-C	5.41	116.64	108.96
1	A	602	THR	N-CA-C	-5.36	98.65	108.02
1	A	187	ASN	CA-C-N	-5.34	114.31	119.87
1	A	187	ASN	C-N-CA	-5.34	114.31	119.87
1	A	430	LEU	N-CA-C	-5.28	106.80	113.18
1	B	430	LEU	N-CA-C	-5.27	106.80	113.18
1	B	677	GLY	N-CA-C	-5.24	106.44	112.73
1	B	464	LYS	N-CA-C	5.20	116.75	111.14
1	A	464	LYS	N-CA-C	5.19	116.63	110.97
1	A	555	VAL	N-CA-C	5.16	120.07	109.34
1	A	454	GLY	N-CA-C	-5.11	104.50	112.58
1	A	677	GLY	N-CA-C	-5.11	106.60	112.73
1	A	465	THR	N-CA-C	5.11	119.56	113.23
1	B	660	THR	N-CA-C	5.06	118.47	109.96
1	B	555	VAL	N-CA-C	5.05	119.84	109.34
1	B	454	GLY	N-CA-C	-5.03	104.64	112.58

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	6417	0	6412	201	0
1	B	6423	0	6417	191	0
2	A	15	0	15	0	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
4	A	30	0	18	0	0
5	A	27	0	20	0	0
6	B	8	0	14	0	0
7	A	307	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	240	0	0	18	0
All	All	13497	0	12910	386	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 15.

All (386) 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	1.36	1.05
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.38	1.03
1:B:110:GLU:HA	7:B:2505:HOH:O	1.65	0.93
1:B:113:TYR:HB3	7:B:2505:HOH:O	1.69	0.93
1:A:213:THR:HB	7:A:2504:HOH:O	1.70	0.91
1:A:710:ILE:HD13	7:A:2205:HOH:O	1.72	0.89
1:A:798:ASN:HB3	7:A:2061:HOH:O	1.72	0.87
1:A:247:ARG:HD3	7:A:2472:HOH:O	1.76	0.85
1:A:547:GLN:O	1:A:551:THR:HG23	1.76	0.85
1:B:547:GLN:O	1:B:551:THR:HG23	1.77	0.84
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.10	0.82
1:A:645:LEU:HD13	1:A:652:LEU:HD11	1.61	0.81
1:A:469:LYS:HG3	7:A:2489:HOH:O	1.81	0.79
1:B:645:LEU:HD13	1:B:652:LEU:HD11	1.62	0.79
1:A:645:LEU:CD1	1:A:652:LEU:HD11	2.13	0.79
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.13	0.78
1:B:645:LEU:CD1	1:B:652:LEU:HD11	2.15	0.76
1:A:278:VAL:HG21	1:B:266:VAL:HG11	1.69	0.74
1:B:197:MET:HE2	1:B:224:LEU:HD13	1.70	0.73
1:A:279:LEU:HD22	7:A:2498:HOH:O	1.89	0.72
1:A:198:LEU:HD21	1:A:309:ARG:NH2	2.05	0.71
1:B:599:VAL:HB	7:B:2328:HOH:O	1.91	0.70
1:A:205:LYS:HB2	7:A:2292:HOH:O	1.91	0.70
1:A:279:LEU:CD2	7:A:2498:HOH:O	2.41	0.69
1:B:198:LEU:HD21	1:B:309:ARG:NH2	2.08	0.69
1:A:130:GLY:O	7:A:2498:HOH:O	2.11	0.68
1:A:146:SER:O	1:A:150:LEU:HD13	1.92	0.68
1:B:615:MET:HE3	1:B:618:MET:HB2	1.76	0.68
1:A:197:MET:HE2	1:A:224:LEU:HD13	1.73	0.68
1:B:433:GLU:HG2	1:B:437:LYS:HE2	1.76	0.68
1:A:433:GLU:HG2	1:A:437:LYS:HE2	1.76	0.67
1:B:29:LYS:HG2	1:B:33:ARG:NH2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG11	1:B:278:VAL:HG21	1.76	0.67
1:A:29:LYS:HG2	1:A:33:ARG:NH2	2.09	0.67
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.76	0.67
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.77	0.67
1:B:615:MET:CE	1:B:761:ILE:HG12	2.21	0.67
1:A:532:ARG:HB2	1:A:532:ARG:HH11	1.60	0.67
1:B:532:ARG:HH11	1:B:532:ARG:HB2	1.58	0.67
1:B:455:VAL:H	1:B:459:HIS:HD2	1.43	0.66
1:A:615:MET:CE	1:A:761:ILE:HG12	2.20	0.66
1:A:594:PRO:HG3	1:A:635:MET:SD	2.34	0.66
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.29	0.66
1:B:146:SER:O	1:B:150:LEU:HD13	1.95	0.66
1:A:325:VAL:HG12	1:A:327:ASP:H	1.62	0.65
1:A:534:LEU:HD23	7:A:2061:HOH:O	1.94	0.65
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.77	0.65
1:B:192:SER:HB3	7:B:2004:HOH:O	1.96	0.65
1:B:415:VAL:HG22	1:B:425:LEU:HD11	1.79	0.65
1:B:594:PRO:HG3	1:B:635:MET:SD	2.37	0.65
1:A:278:VAL:HG21	1:B:266:VAL:CG1	2.26	0.64
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.30	0.64
1:A:615:MET:HE3	1:A:618:MET:HB2	1.78	0.64
1:A:415:VAL:HG22	1:A:425:LEU:HD11	1.79	0.64
1:A:409:LYS:O	1:A:413:ARG:HG2	1.97	0.64
1:A:455:VAL:H	1:A:459:HIS:HD2	1.43	0.64
1:B:469:LYS:O	1:B:473:GLU:HG3	1.97	0.63
1:A:278:VAL:CG2	1:B:266:VAL:HG11	2.28	0.63
1:B:828:GLU:HG3	1:B:829:PRO:HD2	1.80	0.63
1:A:386:ARG:NH2	1:A:438:ARG:HD2	2.14	0.63
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.81	0.62
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.80	0.62
1:B:386:ARG:NH2	1:B:438:ARG:HD2	2.15	0.62
1:A:118:ASP:OD1	1:A:121:GLU:HG3	2.00	0.62
1:B:204:GLY:C	1:B:205:LYS:HD2	2.24	0.61
1:A:366:GLU:HA	7:A:2453:HOH:O	2.00	0.61
1:B:409:LYS:O	1:B:413:ARG:HG2	1.99	0.61
1:A:764:MET:SD	1:A:765:LEU:HD12	2.41	0.61
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.26	0.61
1:A:469:LYS:O	1:A:473:GLU:HG3	2.00	0.60
1:B:118:ASP:OD1	1:B:121:GLU:HG3	2.02	0.60
1:B:308:ILE:HD12	1:B:352:ILE:HG21	1.84	0.60
1:A:316:PHE:N	1:A:316:PHE:CD2	2.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLY:C	1:A:205:LYS:HD2	2.27	0.60
1:A:421:ASP:OD1	1:A:424:ARG:HD2	2.02	0.59
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.27	0.59
1:B:814:ASP:O	1:B:818:LYS:HG3	2.03	0.59
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.85	0.59
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.85	0.59
1:A:399:HIS:O	1:A:403:ILE:HG13	2.01	0.59
1:B:124:GLU:OE2	7:B:2413:HOH:O	2.16	0.58
1:B:470:ASP:O	1:B:474:LEU:HD13	2.03	0.58
1:A:369:GLN:HB2	7:A:2453:HOH:O	2.02	0.58
1:A:423:ASP:O	1:A:427:ARG:HG3	2.03	0.58
1:B:543:LEU:HB3	7:B:2406:HOH:O	2.04	0.58
1:A:233:TYR:CZ	1:A:512:VAL:HG11	2.39	0.58
1:A:814:ASP:O	1:A:818:LYS:HG3	2.04	0.57
1:B:399:HIS:O	1:B:403:ILE:HG13	2.03	0.57
1:B:386:ARG:HB3	1:B:438:ARG:HD3	1.85	0.57
1:B:422:VAL:HG23	1:B:423:ASP:N	2.19	0.57
1:B:433:GLU:CG	1:B:437:LYS:HE2	2.34	0.57
1:A:386:ARG:HB3	1:A:438:ARG:HD3	1.86	0.57
1:A:433:GLU:CG	1:A:437:LYS:HE2	2.35	0.57
1:B:785:ASP:O	1:B:789:GLN:HG2	2.05	0.57
1:A:266:VAL:CG1	1:B:278:VAL:HG21	2.34	0.56
1:A:325:VAL:HA	7:A:2508:HOH:O	2.04	0.56
1:A:330:PRO:HB2	7:A:2416:HOH:O	2.05	0.56
1:A:735:LEU:HD23	1:A:777:TYR:HD2	1.70	0.56
1:B:81:ARG:NH2	7:B:2240:HOH:O	2.35	0.56
1:B:592:LYS:O	1:B:594:PRO:HD3	2.06	0.56
1:A:470:ASP:O	1:A:474:LEU:HD13	2.05	0.56
1:B:713:MET:HE1	1:B:772:LYS:HD3	1.87	0.56
1:B:752:PRO:HG2	7:B:2354:HOH:O	2.05	0.56
1:B:753:LYS:HG2	7:B:2354:HOH:O	2.06	0.56
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.46	0.56
1:A:266:VAL:HG11	1:B:278:VAL:CG2	2.37	0.56
1:B:675:GLY:O	1:B:679:MET:HE3	2.07	0.55
1:A:422:VAL:HG23	1:A:423:ASP:N	2.21	0.55
1:B:538:LYS:O	1:B:542:LYS:HG3	2.07	0.55
1:B:309:ARG:NH2	7:B:2450:HOH:O	2.33	0.55
1:B:422:VAL:CG2	1:B:423:ASP:N	2.71	0.54
1:A:95:LEU:HD22	1:A:99:MET:HE2	1.89	0.54
1:A:592:LYS:O	1:A:594:PRO:HD3	2.07	0.54
1:A:785:ASP:O	1:A:789:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:ASN:C	1:B:826:ASN:HD22	2.14	0.54
1:B:423:ASP:O	1:B:427:ARG:HG3	2.07	0.54
1:A:314:SER:O	1:A:315:LYS:HB3	2.07	0.54
1:B:421:ASP:OD1	1:B:424:ARG:HD2	2.08	0.54
1:B:532:ARG:HB2	1:B:532:ARG:NH1	2.22	0.53
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.08	0.53
1:B:118:ASP:HA	7:B:2363:HOH:O	2.07	0.53
1:A:132:GLY:N	7:A:2498:HOH:O	2.42	0.53
1:B:314:SER:O	1:B:315:LYS:HB3	2.07	0.53
1:A:106:ASN:N	1:A:106:ASN:HD22	2.06	0.53
1:A:532:ARG:HB2	1:A:532:ARG:NH1	2.23	0.53
1:A:538:LYS:O	1:A:542:LYS:HG3	2.08	0.53
1:B:106:ASN:N	1:B:106:ASN:HD22	2.07	0.53
1:A:422:VAL:CG2	1:A:423:ASP:N	2.71	0.53
1:A:494:LEU:HD23	1:A:494:LEU:C	2.34	0.53
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.91	0.53
1:B:735:LEU:HD23	1:B:777:TYR:HD2	1.73	0.53
1:A:316:PHE:N	1:A:316:PHE:HD2	2.05	0.52
1:A:713:MET:HE1	1:A:772:LYS:HD3	1.91	0.52
1:A:459:HIS:O	1:A:463:VAL:HG23	2.10	0.52
1:A:206:VAL:HG13	7:A:2504:HOH:O	2.08	0.52
1:A:675:GLY:O	1:A:679:MET:HE3	2.08	0.52
1:B:93:ARG:HG2	1:B:126:GLU:HG2	1.92	0.52
1:B:697:VAL:O	1:B:701:GLU:HG3	2.10	0.52
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.50	0.52
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.40	0.52
1:B:308:ILE:HD12	1:B:352:ILE:HD13	1.92	0.52
1:A:565:VAL:HG22	1:A:604:ILE:HB	1.91	0.51
1:A:308:ILE:HD12	1:A:352:ILE:HG21	1.91	0.51
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.46	0.51
1:B:459:HIS:O	1:B:463:VAL:HG23	2.10	0.51
1:B:410:HIS:O	1:B:414:ILE:HD13	2.09	0.51
1:A:22:GLU:HB3	1:A:62:HIS:HE1	1.76	0.51
1:A:208:HIS:ND1	1:A:213:THR:HG22	2.26	0.51
1:A:735:LEU:N	1:A:735:LEU:CD1	2.73	0.51
1:B:208:HIS:ND1	1:B:213:THR:HG22	2.25	0.51
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.93	0.51
1:B:735:LEU:CD1	1:B:735:LEU:N	2.74	0.51
1:B:246:ALA:O	1:B:247:ARG:HD2	2.11	0.51
1:B:300:VAL:CG1	1:B:345:ALA:HA	2.41	0.50
1:A:410:HIS:O	1:A:414:ILE:HD13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:TRP:HA	1:B:238:VAL:HB	1.93	0.50
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.92	0.50
1:A:136:LEU:HD23	1:A:136:LEU:C	2.36	0.50
1:A:693:ASP:O	1:A:696:ASN:HB2	2.12	0.50
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.93	0.50
1:A:826:ASN:C	1:A:826:ASN:HD22	2.19	0.50
1:B:693:ASP:O	1:B:696:ASN:HB2	2.10	0.50
1:B:764:MET:SD	1:B:765:LEU:HD12	2.52	0.50
1:B:572:GLU:HG3	1:B:613:TYR:OH	2.11	0.50
1:A:693:ASP:O	1:A:694:GLY:C	2.54	0.50
1:A:795:LYS:HB2	7:A:2122:HOH:O	2.11	0.50
1:B:72:GLN:HE21	1:B:76:ASP:CG	2.19	0.50
1:A:411:LEU:O	1:A:415:VAL:HG23	2.12	0.50
1:A:697:VAL:O	1:A:701:GLU:HG3	2.12	0.50
1:A:308:ILE:O	1:A:312:LYS:HG3	2.12	0.49
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.94	0.49
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.94	0.49
1:B:592:LYS:C	1:B:592:LYS:HE2	2.38	0.49
1:B:693:ASP:O	1:B:694:GLY:C	2.54	0.49
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.49
1:A:592:LYS:HE2	1:A:592:LYS:C	2.38	0.49
1:B:577:LEU:CD1	1:B:765:LEU:HD11	2.42	0.49
1:A:198:LEU:HD21	1:A:309:ARG:CZ	2.42	0.49
1:B:411:LEU:O	1:B:415:VAL:HG23	2.12	0.49
1:A:66:ARG:CD	1:A:236:ASN:HA	2.42	0.49
1:A:828:GLU:HG3	1:A:829:PRO:HD2	1.94	0.49
1:B:826:ASN:O	1:B:826:ASN:ND2	2.38	0.49
1:A:737:GLU:O	1:A:741:VAL:HG23	2.12	0.49
1:B:737:GLU:O	1:B:741:VAL:HG23	2.12	0.49
1:A:246:ALA:O	1:A:247:ARG:HD2	2.12	0.48
1:B:45:VAL:HG12	1:B:45:VAL:O	2.11	0.48
1:A:645:LEU:HD11	1:A:652:LEU:HD11	1.90	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.95	0.48
1:A:369:GLN:NE2	7:A:2453:HOH:O	2.46	0.48
1:B:66:ARG:CD	1:B:236:ASN:HA	2.43	0.48
1:B:724:LYS:O	1:B:724:LYS:HD3	2.13	0.48
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.49	0.48
1:B:198:LEU:HD21	1:B:309:ARG:CZ	2.44	0.48
1:B:652:LEU:HD13	1:B:652:LEU:O	2.14	0.48
1:A:556:LYS:HD3	1:A:557:ILE:N	2.28	0.48
1:A:65:GLY:O	1:A:69:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:OD1	1:A:281:PRO:HA	2.14	0.48
1:A:689:ILE:HG23	1:A:689:ILE:O	2.14	0.48
1:A:45:VAL:HG12	1:A:45:VAL:O	2.14	0.48
1:B:205:LYS:HG3	7:B:2302:HOH:O	2.13	0.47
1:B:689:ILE:O	1:B:689:ILE:HG23	2.14	0.47
1:A:301:ALA:O	1:A:305:GLN:HG3	2.13	0.47
1:A:386:ARG:HA	1:A:439:ILE:O	2.14	0.47
1:A:724:LYS:O	1:A:724:LYS:HD3	2.14	0.47
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.44	0.47
1:B:65:GLY:O	1:B:69:ARG:HG3	2.15	0.47
1:B:645:LEU:HD11	1:B:652:LEU:HD11	1.94	0.47
1:A:545:PHE:O	1:A:548:PHE:HB3	2.14	0.47
1:A:577:LEU:CD1	1:A:765:LEU:HD11	2.44	0.47
1:A:261:ASP:N	7:A:2495:HOH:O	2.47	0.47
1:A:414:ILE:CG2	1:A:425:LEU:HD23	2.45	0.47
1:A:382:GLU:CD	1:A:382:GLU:H	2.23	0.47
1:B:532:ARG:NH1	1:B:532:ARG:CB	2.78	0.47
1:B:655:LYS:O	1:B:658:PRO:HD2	2.15	0.47
1:B:692:MET:HE2	1:B:710:ILE:HG21	1.97	0.47
1:B:615:MET:HE3	1:B:615:MET:O	2.15	0.47
1:B:746:ASP:HB2	1:B:762:ILE:HG13	1.97	0.47
1:A:203:TYR:HE2	1:A:394:LYS:HD2	1.80	0.47
1:A:511:TYR:N	7:A:2148:HOH:O	2.47	0.47
1:A:746:ASP:HB2	1:A:762:ILE:HG13	1.97	0.47
1:A:132:GLY:O	7:A:2498:HOH:O	2.20	0.47
1:A:532:ARG:NH1	1:A:532:ARG:CB	2.78	0.47
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.50	0.47
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	0.46
1:A:424:ARG:HH22	1:A:474:LEU:CD1	2.28	0.46
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.49	0.46
1:A:293:LEU:HG	1:A:395:LEU:HD23	1.96	0.46
1:A:571:HIS:H	1:A:576:GLN:NE2	2.12	0.46
1:B:301:ALA:O	1:B:305:GLN:HG3	2.15	0.46
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.50	0.46
1:B:382:GLU:CD	1:B:382:GLU:H	2.22	0.46
1:A:402:ILE:O	1:A:406:ILE:HG13	2.15	0.46
1:A:576:GLN:NE2	1:A:576:GLN:H	2.13	0.46
1:B:136:LEU:C	1:B:136:LEU:HD23	2.40	0.46
1:B:732:TYR:CE1	1:B:739:LYS:HA	2.51	0.46
1:A:398:ARG:O	1:A:402:ILE:HG13	2.16	0.46
1:A:592:LYS:O	1:A:592:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ASP:O	1:A:636:VAL:HG22	2.15	0.46
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.51	0.46
1:A:732:TYR:CE1	1:A:739:LYS:HA	2.51	0.46
1:A:826:ASN:O	1:A:826:ASN:ND2	2.39	0.46
1:B:754:GLN:HB3	1:B:757:LEU:HB2	1.96	0.46
1:A:615:MET:HE3	1:A:615:MET:O	2.15	0.46
1:B:402:ILE:O	1:B:406:ILE:HG13	2.16	0.46
1:B:566:GLN:HA	7:B:2012:HOH:O	2.15	0.46
1:A:315:LYS:O	1:A:316:PHE:C	2.58	0.46
1:A:575:ARG:HD3	1:A:666:ILE:O	2.15	0.46
1:B:576:GLN:H	1:B:576:GLN:NE2	2.13	0.46
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.98	0.45
1:B:432:GLU:O	1:B:437:LYS:HA	2.17	0.45
1:B:494:LEU:C	1:B:494:LEU:HD23	2.40	0.45
1:B:738:LEU:HB2	1:B:777:TYR:CE2	2.51	0.45
1:A:715:ILE:HG23	1:A:716:ASP:N	2.30	0.45
1:B:133:ASN:OD1	1:B:281:PRO:HA	2.16	0.45
1:B:216:ILE:HB	7:B:2168:HOH:O	2.16	0.45
1:B:648:TYR:HD1	1:B:652:LEU:HD12	1.81	0.45
1:B:728:ALA:HB1	1:B:774:PHE:CD1	2.51	0.45
1:B:633:ASP:O	1:B:636:VAL:HG22	2.16	0.45
1:A:754:GLN:HB3	1:A:757:LEU:HB2	1.97	0.45
1:B:414:ILE:CG2	1:B:425:LEU:HD23	2.45	0.45
1:B:433:GLU:HG3	1:B:437:LYS:HG2	1.99	0.45
1:B:715:ILE:HG23	1:B:716:ASP:N	2.31	0.45
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.98	0.45
1:B:592:LYS:O	1:B:592:LYS:HE2	2.15	0.45
1:B:636:VAL:HG23	1:B:637:GLY:N	2.32	0.45
1:A:389:VAL:HG22	1:A:437:LYS:O	2.16	0.45
1:A:469:LYS:HZ3	1:A:473:GLU:CD	2.25	0.45
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.99	0.45
1:B:81:ARG:HD3	1:B:155:TYR:HE2	1.82	0.45
1:B:545:PHE:O	1:B:548:PHE:HB3	2.16	0.45
1:A:525:LEU:HD23	1:A:802:LEU:HD23	1.99	0.45
1:A:648:TYR:HD1	1:A:652:LEU:HD12	1.82	0.45
1:B:571:HIS:H	1:B:576:GLN:NE2	2.15	0.45
1:B:769:ASP:OD1	1:B:769:ASP:C	2.58	0.45
1:A:732:TYR:CD1	1:A:739:LYS:HA	2.52	0.45
1:B:95:LEU:HD22	1:B:99:MET:HE2	1.98	0.45
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.92	0.45
1:B:438:ARG:HE	1:B:438:ARG:HB3	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.82	0.44
1:B:81:ARG:HD3	1:B:155:TYR:CE2	2.52	0.44
1:B:315:LYS:O	1:B:315:LYS:HG3	2.17	0.44
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.99	0.44
1:A:316:PHE:HD2	1:A:316:PHE:H	1.64	0.44
1:B:652:LEU:HD13	1:B:652:LEU:C	2.43	0.44
1:B:732:TYR:CD1	1:B:739:LYS:HA	2.52	0.44
1:A:415:VAL:HG22	1:A:425:LEU:CD1	2.48	0.44
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.52	0.44
1:B:308:ILE:O	1:B:312:LYS:HG3	2.17	0.44
1:A:241:MET:HE3	1:A:243:LEU:HD22	1.99	0.44
1:B:106:ASN:HB3	7:B:2216:HOH:O	2.17	0.44
1:B:556:LYS:HD3	1:B:557:ILE:N	2.32	0.44
1:B:487:THR:HA	1:B:488:PRO:HD3	1.88	0.44
1:A:336:GLN:OE1	1:A:825:TRP:NE1	2.45	0.43
1:A:558:ASN:HB3	1:A:561:SER:HB3	2.00	0.43
1:B:98:THR:O	1:B:102:LEU:HB2	2.18	0.43
1:B:424:ARG:HH22	1:B:474:LEU:CD1	2.30	0.43
1:A:81:ARG:HD3	1:A:155:TYR:CE2	2.53	0.43
1:A:308:ILE:HD12	1:A:352:ILE:HD13	2.00	0.43
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.99	0.43
1:A:769:ASP:OD1	1:A:769:ASP:C	2.60	0.43
1:B:567:VAL:HA	1:B:606:GLY:O	2.18	0.43
1:B:575:ARG:HD3	1:B:666:ILE:O	2.18	0.43
1:B:36:HIS:O	1:B:40:VAL:HA	2.19	0.43
1:B:386:ARG:HA	1:B:439:ILE:O	2.17	0.43
1:A:438:ARG:HE	1:A:438:ARG:HB3	1.62	0.43
1:B:135:GLY:HA3	7:B:2008:HOH:O	2.18	0.43
1:A:566:GLN:HA	7:A:2057:HOH:O	2.18	0.43
1:B:389:VAL:HG22	1:B:437:LYS:O	2.17	0.43
1:B:415:VAL:HG22	1:B:425:LEU:CD1	2.47	0.43
1:B:576:GLN:H	1:B:576:GLN:CD	2.27	0.43
1:B:555:VAL:HG12	1:B:556:LYS:N	2.33	0.43
1:A:432:GLU:O	1:A:437:LYS:HA	2.19	0.43
1:A:756:ASP:O	1:A:759:LYS:HB2	2.18	0.43
1:B:417:LEU:C	1:B:419:PRO:HD3	2.44	0.43
1:B:756:ASP:O	1:B:759:LYS:HB2	2.18	0.43
1:A:198:LEU:CD2	1:A:309:ARG:NH2	2.78	0.43
1:B:311:PHE:CE1	1:B:329:PHE:HA	2.54	0.43
1:B:708:LEU:HG	7:B:2209:HOH:O	2.18	0.43
1:A:636:VAL:HG23	1:A:637:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HG12	1:B:646:GLU:HB3	2.01	0.43
1:B:336:GLN:OE1	1:B:825:TRP:NE1	2.47	0.43
1:B:792:MET:O	1:B:794:PRO:HD3	2.18	0.43
1:B:828:GLU:CG	1:B:829:PRO:HD2	2.47	0.43
1:A:567:VAL:HA	1:A:606:GLY:O	2.19	0.42
1:B:374:TYR:CG	1:B:445:CYS:HB3	2.54	0.42
1:A:24:VAL:O	1:A:28:LYS:HG3	2.18	0.42
1:B:754:GLN:N	1:B:755:PRO:HD3	2.34	0.42
1:A:360:PRO:HB2	7:A:2441:HOH:O	2.19	0.42
1:A:417:LEU:C	1:A:419:PRO:HD3	2.44	0.42
1:A:792:MET:O	1:A:794:PRO:HD3	2.19	0.42
1:B:325:VAL:HA	7:B:2535:HOH:O	2.19	0.42
1:A:314:SER:C	1:A:316:PHE:H	2.28	0.42
1:A:818:LYS:HD3	7:A:2547:HOH:O	2.20	0.42
1:A:761:ILE:O	1:A:765:LEU:HD13	2.20	0.42
1:A:74:TYR:HB3	1:A:81:ARG:NH1	2.34	0.42
1:B:558:ASN:HB3	1:B:561:SER:HB3	2.01	0.42
1:B:615:MET:CE	1:B:618:MET:HB2	2.48	0.42
1:A:555:VAL:HG12	1:A:556:LYS:N	2.33	0.42
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.01	0.42
1:A:735:LEU:HD23	1:A:777:TYR:CD2	2.52	0.42
1:A:36:HIS:O	1:A:40:VAL:HA	2.19	0.42
1:A:210:ASN:ND2	7:A:2270:HOH:O	2.53	0.42
1:A:554:LYS:O	1:A:555:VAL:O	2.38	0.42
1:A:735:LEU:N	1:A:735:LEU:HD12	2.35	0.42
1:B:233:TYR:CD2	1:B:513:LYS:HE3	2.55	0.42
1:B:713:MET:HB3	1:B:717:ASP:HB2	2.02	0.42
1:A:557:ILE:O	1:A:559:PRO:HD3	2.20	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.20	0.42
1:B:42:ASP:C	1:B:42:ASP:OD2	2.62	0.42
1:A:98:THR:O	1:A:102:LEU:HB2	2.18	0.41
1:B:528:ASP:CG	1:B:795:LYS:HZ3	2.28	0.41
1:B:657:ILE:HB	1:B:658:PRO:HD3	2.02	0.41
1:A:300:VAL:HG13	1:A:345:ALA:HA	2.02	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.86	0.41
1:B:761:ILE:O	1:B:765:LEU:HD13	2.19	0.41
1:A:433:GLU:HG3	1:A:437:LYS:HG2	2.01	0.41
1:B:206:VAL:HG11	1:B:401:GLU:CD	2.45	0.41
1:A:81:ARG:HD3	1:A:155:TYR:HE2	1.86	0.41
1:A:590:ILE:HA	7:A:2392:HOH:O	2.21	0.41
1:B:22:GLU:HA	1:B:22:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ASP:O	1:B:284:ASN:HB2	2.20	0.41
1:A:576:GLN:H	1:A:576:GLN:CD	2.27	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.36	0.41
1:B:735:LEU:HD23	1:B:777:TYR:CD2	2.54	0.41
1:A:315:LYS:O	1:A:315:LYS:HG3	2.21	0.41
1:B:786:LYS:HB3	1:B:786:LYS:HE2	1.72	0.41
1:A:633:ASP:HA	1:A:634:PRO:HD3	1.91	0.41
1:B:525:LEU:HD23	1:B:802:LEU:HD23	2.03	0.41
1:A:652:LEU:HD13	1:A:652:LEU:C	2.46	0.41
1:B:233:TYR:CZ	1:B:512:VAL:HG11	2.56	0.41
1:B:636:VAL:CG2	1:B:637:GLY:N	2.84	0.41
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.51	0.41
1:B:246:ALA:O	1:B:273:GLU:HG2	2.21	0.41
1:A:281:PRO:HD2	7:A:2410:HOH:O	2.20	0.40
1:A:291:LEU:O	1:A:295:GLN:HG3	2.21	0.40
1:A:601:ARG:HG3	7:A:2212:HOH:O	2.21	0.40
1:B:203:TYR:HE2	1:B:394:LYS:HD2	1.86	0.40
1:B:561:SER:HA	1:B:600:PRO:HG2	2.03	0.40
1:A:418:PHE:N	1:A:419:PRO:HD3	2.36	0.40
1:A:655:LYS:O	1:A:658:PRO:HD2	2.21	0.40
1:B:282:ASN:HB3	1:B:285:PHE:HB3	2.04	0.40
1:B:555:VAL:CG1	1:B:556:LYS:N	2.84	0.40
1:B:34:HIS:CE1	1:B:57:HIS:HB3	2.56	0.40
1:B:692:MET:HG3	1:B:697:VAL:HG22	2.03	0.40
1:B:418:PHE:N	1:B:419:PRO:HD3	2.36	0.40
1:B:690:GLY:O	1:B:710:ILE:HA	2.21	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	784/847 (93%)	742 (95%)	39 (5%)	3 (0%)	30	28
1	B	785/847 (93%)	742 (94%)	39 (5%)	4 (0%)	24	22
All	All	1569/1694 (93%)	1484 (95%)	78 (5%)	7 (0%)	30	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	VAL
1	B	555	VAL
1	A	554	LYS
1	B	554	LYS
1	A	342	PRO
1	B	342	PRO
1	B	694	GLY

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

6 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	902	-	7,7,7	0.71	0	9,10,10	0.77	0
4	700	A	862	-	31,33,33	1.93	10 (32%)	44,47,47	1.71	8 (18%)
5	RBF	A	859	-	29,29,29	1.61	9 (31%)	42,43,43	2.11	14 (33%)
3	PLP	A	860	1	15,15,16	2.19	6 (40%)	21,22,23	1.35	3 (14%)
2	NBG	A	861	-	15,15,15	1.28	3 (20%)	21,21,21	1.22	1 (4%)
3	PLP	B	860	1	15,15,16	2.05	3 (20%)	21,22,23	0.91	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
6	MRD	B	902	-	-	2/5/5/5	-
4	700	A	862	-	-	0/22/32/32	0/4/4/4
5	RBF	A	859	-	-	2/14/14/14	0/3/3/3
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
3	PLP	B	860	1	-	2/6/6/8	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	860	PLP	C4A-C4	-5.71	1.40	1.51
3	A	860	PLP	C4A-C4	-5.25	1.41	1.51
4	A	862	700	C8-N2	-4.14	1.32	1.38
4	A	862	700	C5-C4	3.65	1.44	1.38
3	B	860	PLP	C3-C2	-3.58	1.37	1.41
3	A	860	PLP	C5A-C5	3.46	1.59	1.50
4	A	862	700	C3-C4	3.24	1.44	1.38
5	A	859	RBF	C8M-C8	3.13	1.56	1.51
5	A	859	RBF	C8-C7	2.87	1.47	1.40
4	A	862	700	C16-C11	2.86	1.44	1.38
4	A	862	700	C13-C12	2.82	1.43	1.38
5	A	859	RBF	C9-C9A	2.71	1.44	1.39
4	A	862	700	C6-C7	2.68	1.52	1.44
2	A	861	NBG	C2-C1	2.67	1.55	1.53
5	A	859	RBF	C5'-C4'	2.60	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	862	700	C15-C14	2.59	1.43	1.38
5	A	859	RBF	C1'-C2'	2.56	1.56	1.52
4	A	862	700	C12-C11	2.51	1.43	1.38
4	A	862	700	O4-C21	-2.50	1.22	1.30
4	A	862	700	C3-C2	2.48	1.42	1.38
3	A	860	PLP	C2-N1	2.33	1.38	1.33
5	A	859	RBF	C1'-N10	2.28	1.53	1.47
5	A	859	RBF	C4'-C3'	-2.26	1.49	1.53
3	A	860	PLP	P-O3P	-2.19	1.46	1.54
5	A	859	RBF	O2-C2	-2.19	1.20	1.24
3	A	860	PLP	C3-C4	2.11	1.44	1.40
5	A	859	RBF	C4A-C4	2.10	1.52	1.44
3	B	860	PLP	P-O3P	-2.07	1.47	1.54
2	A	861	NBG	C3-C2	2.05	1.57	1.52
3	A	860	PLP	C6-N1	2.04	1.38	1.34
2	A	861	NBG	C1-N1	2.01	1.46	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	859	RBF	O5'-C5'-C4'	-6.01	98.52	111.16
4	A	862	700	C1-C6-C7	-5.32	102.44	106.80
5	A	859	RBF	O4'-C4'-C3'	5.09	121.16	109.25
5	A	859	RBF	C10-N1-C2	4.59	126.79	116.85
5	A	859	RBF	O4-C4-C4A	-4.20	115.44	126.53
4	A	862	700	C8-C9-N1	4.12	122.36	116.86
4	A	862	700	C5-C6-C1	3.95	121.57	119.13
2	A	861	NBG	C5-O5-C1	3.92	117.92	112.47
5	A	859	RBF	C5A-C9A-N10	-3.65	114.67	117.97
4	A	862	700	O1-C9-C8	-3.20	116.96	121.09
3	A	860	PLP	O3P-P-O4P	-2.89	99.13	106.67
4	A	862	700	C1-N2-C8	2.88	112.10	109.01
4	A	862	700	O3-C21-C20	-2.85	115.29	122.86
3	A	860	PLP	O3P-P-O2P	2.82	118.38	107.80
4	A	862	700	O4-C21-O3	2.74	130.29	124.08
5	A	859	RBF	C4A-C4-N3	2.72	120.19	113.25
5	A	859	RBF	C7M-C7-C6	2.56	124.08	119.57
5	A	859	RBF	O4'-C4'-C5'	-2.52	103.29	109.03
4	A	862	700	C6-C5-C4	-2.43	117.49	120.40
3	A	860	PLP	C2A-C2-C3	2.32	123.51	120.80
5	A	859	RBF	O4-C4-N3	2.26	124.37	120.11
5	A	859	RBF	O2-C2-N1	2.24	125.51	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	859	RBF	C4A-C10-N1	-2.23	119.13	124.59
5	A	859	RBF	N10-C10-N1	2.16	124.86	118.51
5	A	859	RBF	C4-N3-C2	-2.04	122.03	125.64
5	A	859	RBF	O3'-C3'-C2'	-2.00	104.38	108.93

There are no chirality outliers.

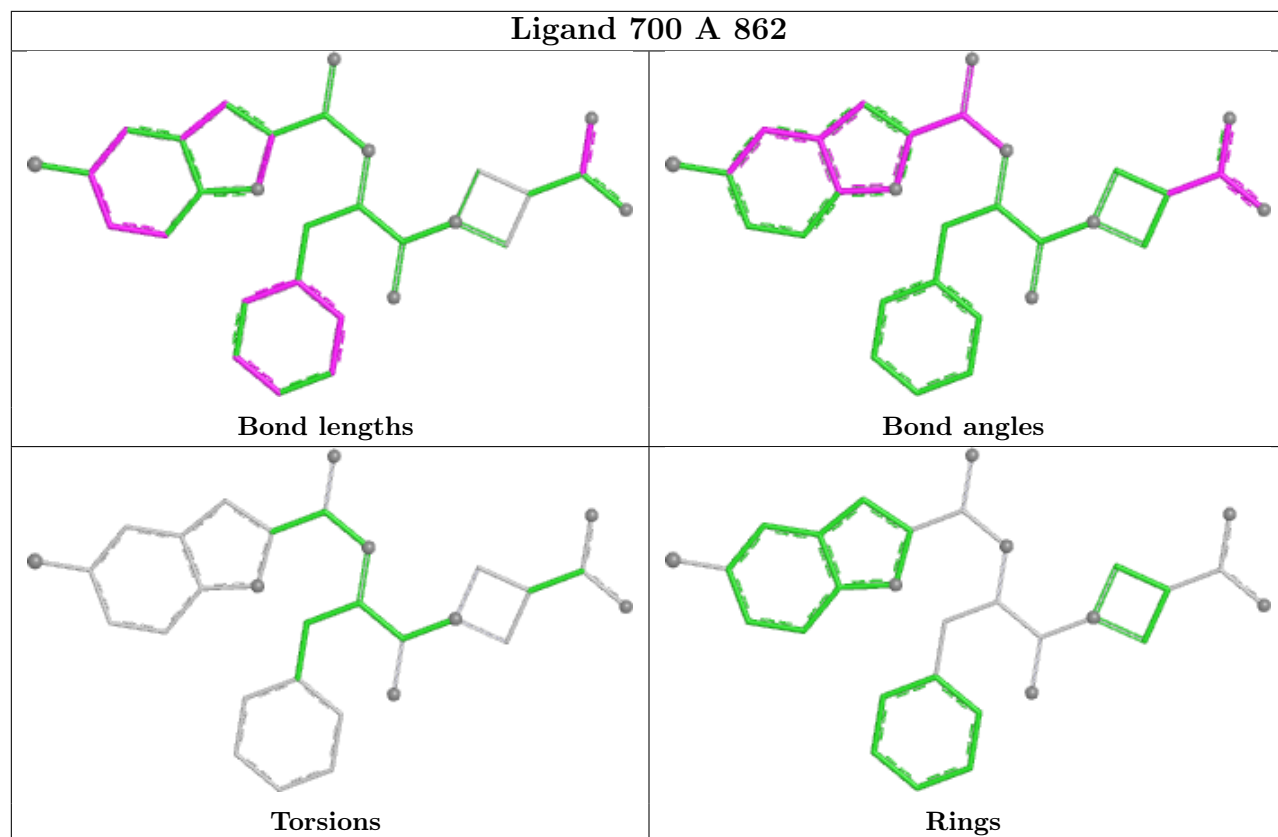
All (6) torsion outliers are listed below:

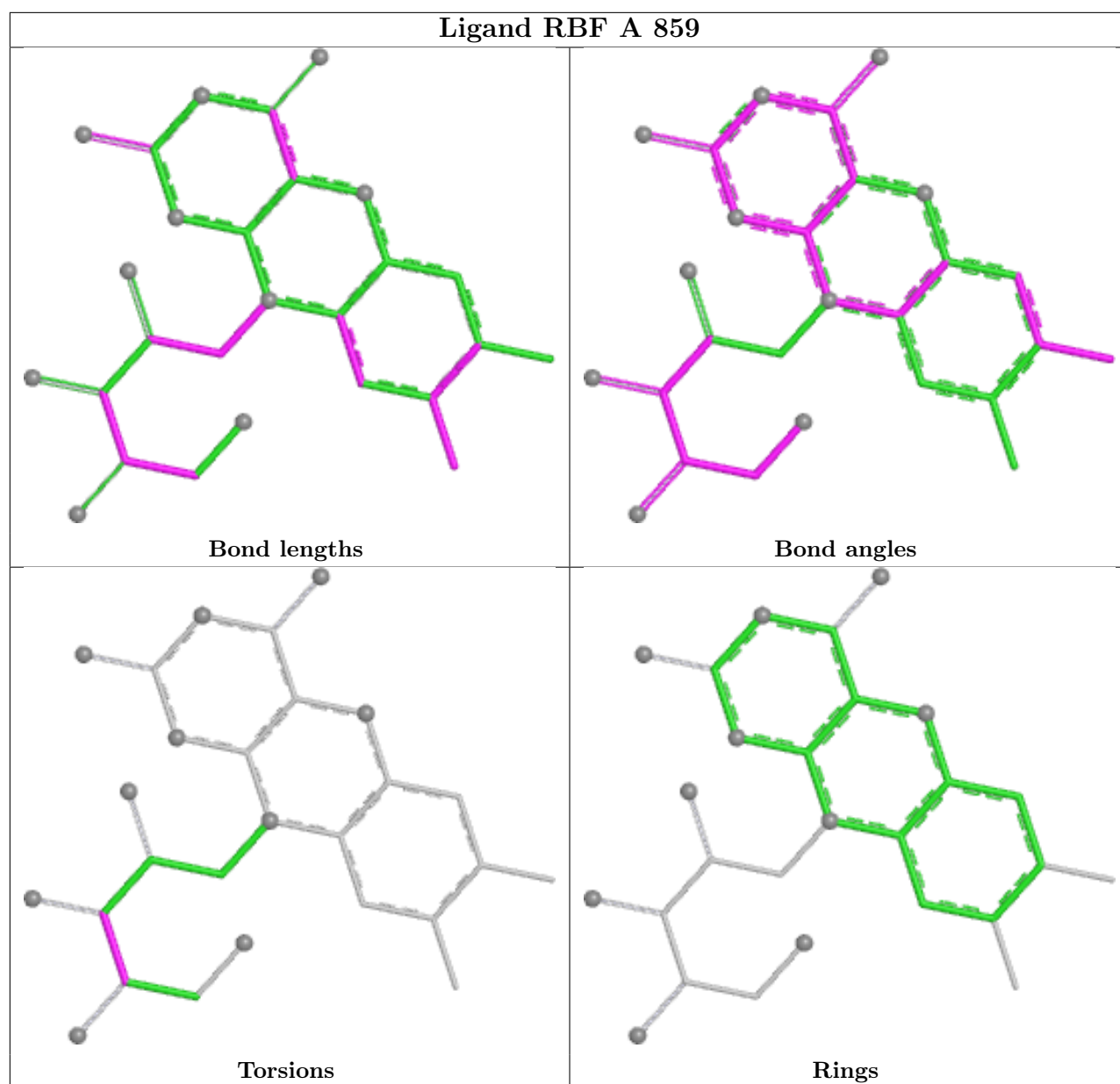
Mol	Chain	Res	Type	Atoms
3	B	860	PLP	C6-C5-C5A-O4P
3	B	860	PLP	C4-C5-C5A-O4P
6	B	902	MRD	C2-C3-C4-O4
6	B	902	MRD	C2-C3-C4-C5
5	A	859	RBF	O3'-C3'-C4'-C5'
5	A	859	RBF	O3'-C3'-C4'-O4'

There are no ring outliers.

No monomer is involved in short contacts.

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.