



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:51 PM UTC

PDB ID : 1EXV / pdb_00001exv
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-403,700
Authors : Rath, V.L.; Ammirati, M.; Danley, D.E.; Ekstrom, J.L.; Hynes, T.R.; Olson, T.V.; Hoover, D.J.
Deposited on : 2000-05-04
Resolution : 2.40 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

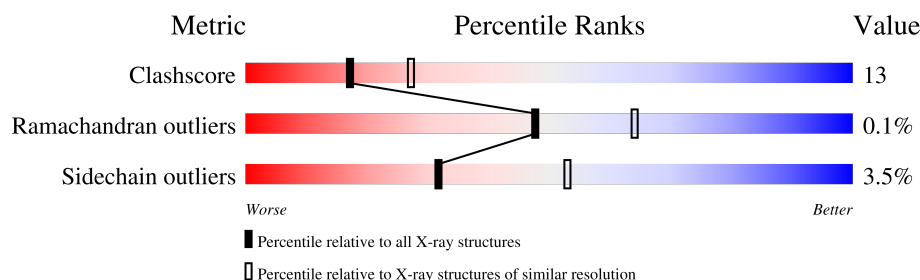
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	1901	X	-	-	-
5	MPD	B	1902	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13223 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.

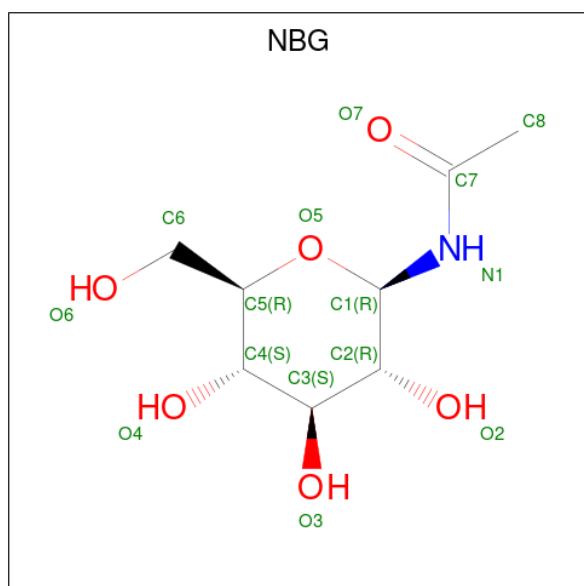
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	0	0
			6377	4098	1083	1167	29			
1	B	786	Total	C	N	O	S	0	0	0
			6377	4098	1083	1167	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	569	ARG	SER	SEE REMARK 999	UNP P06737
B	569	ARG	SER	SEE REMARK 999	UNP P06737

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



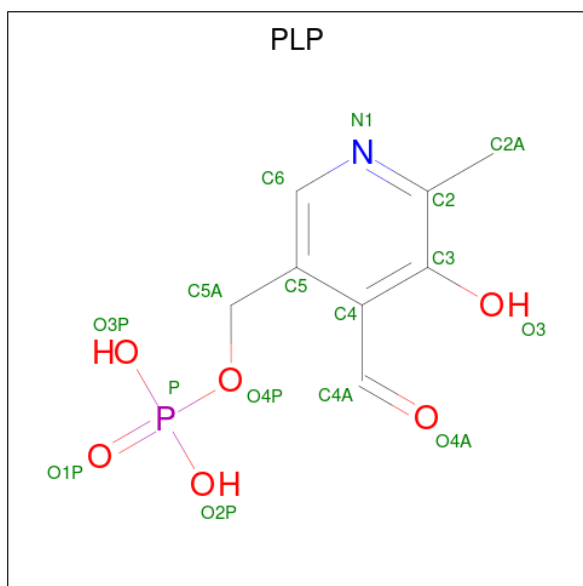
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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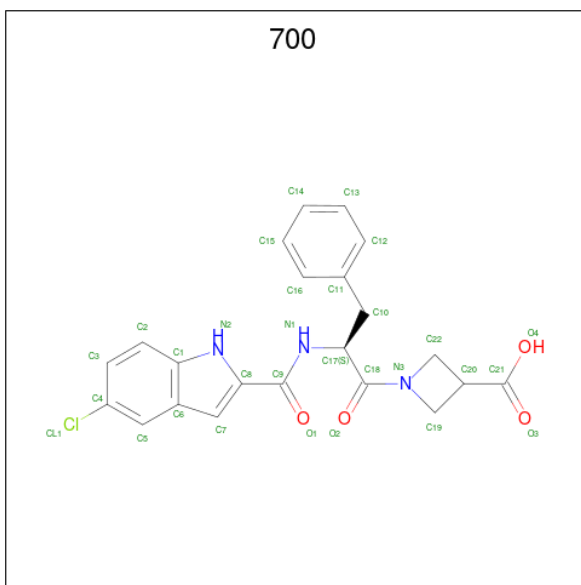
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

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



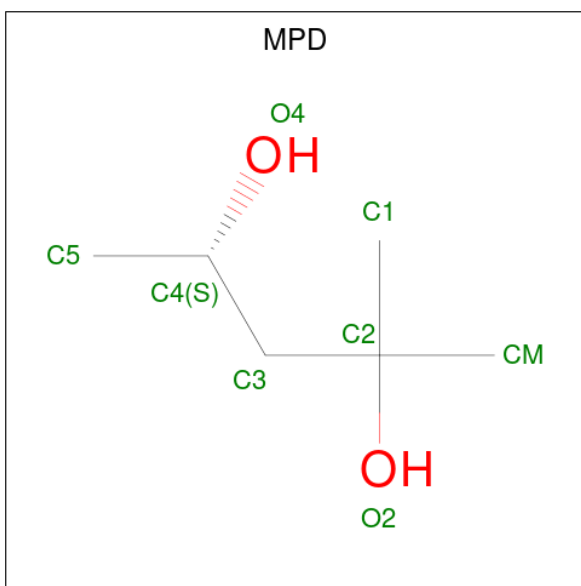
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	174	Total 174	O 174	0	0
6	B	159	Total 159	O 159	0	0

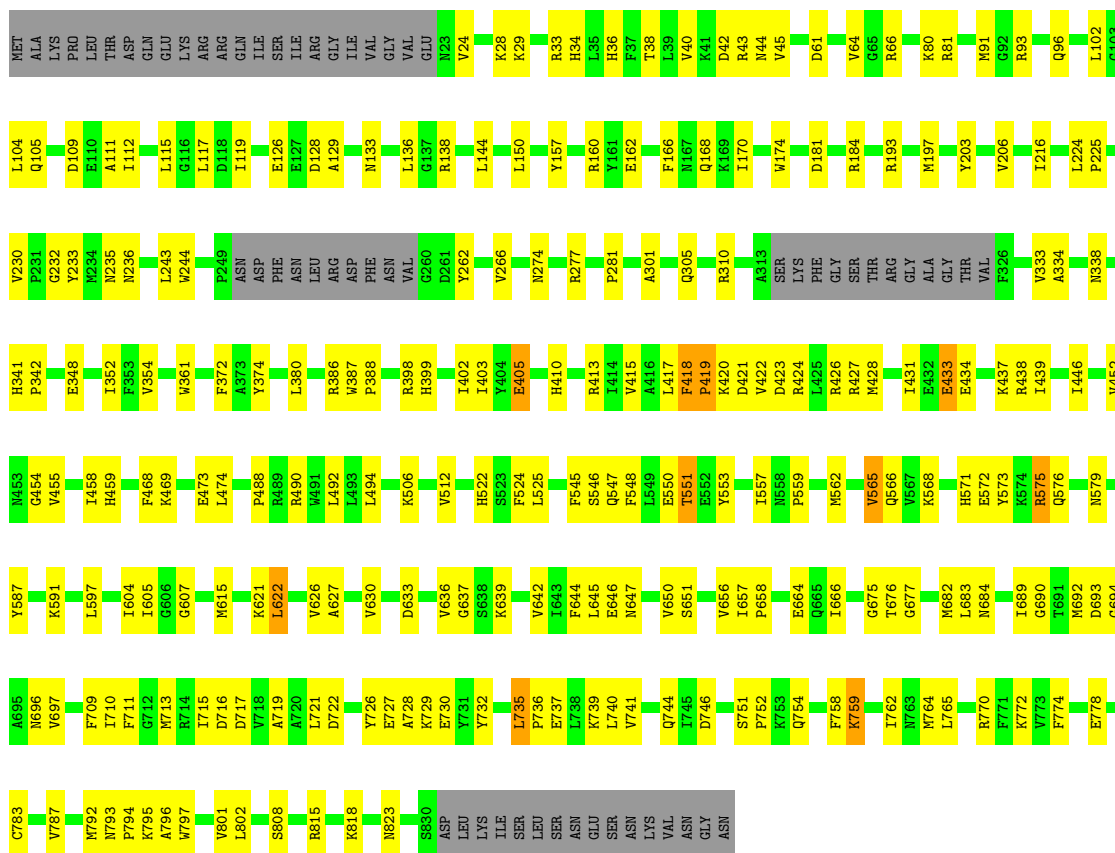
3 Residue-property plots

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.

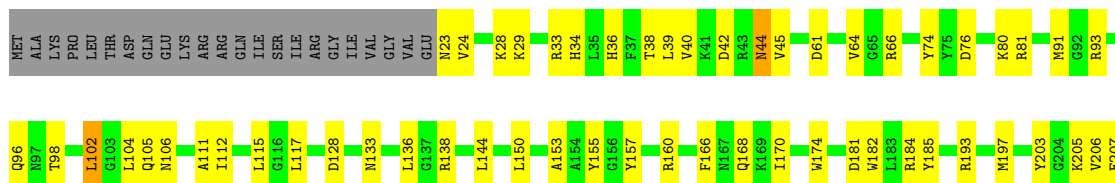
• Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE

Chain A: 



• Molecule 1: LIVER GLYCOGEN PHOSPHORYLASE

Chain B: 



SER	E730	V636	H522	L417	R310	R208
LEU	Y731	G637	S523	F418	R310	T209
SER	Y732	G638	F524	K420	A313	N210
ASN		S638	L525	D421	SER	T211
GLU	L735	K639		V422	LYS	K214
SER	P736		D528	D423	PHE	Q215
ASN	E737	V642	R532	R424	GLY	I216
LYS	L738	F643		L425	SER	D217
VAL	K739	P644	F545	R426	THR	T218
ASN	L740	L645	S546	R427	ARG	Q219
GLY	V741	E646	Q547	M428	GLY	
ASN		N647	F548	I431	ALA	L224
	Q744		L549	E432	GLY	P225
	F745	V650	E550	E433	THR	
	D746	S651	T551	E434	VAL	V230
		L652			F326	P231
	S751	V656	Y553	K437	V333	Q232
	P752	I657	I557	R438	A334	Y233
	K753	P658	N558	I439		M234
	Q754		P559	I446	L337	N235
	F758	E664		V447	N338	N236
	K759	Q665	M562	G448	H341	L243
		I666		S449	P342	W244
	I762	M682	V565	H450		
	H763	L683	Q566	A451	A345	R247
	M764		H571	V452	I346	A248
	L765	I689	E572	N453		P249
		G690	Y573	G454	V354	ASN
	R770	T691	K574	V455	W361	ASP
	F774	M692	R575	I458	F372	PHE
		D693	Q576	H459	A373	ASN
	E778	G694		F468	Y374	LEU
		A695	N579	K469		ARG
	C783	N696	Y587	E473	L380	ASP
	V787	V697		L474	P381	ASN
		E698	K591	E475	L384	ASN
	M792	E702	K592		E385	VAL
	N793		L597	P488	R386	G260
	P794	L708	I604	R489		D261
	K795	F709	I605	W491		Y262
	A796	I710	M615	R490	R398	V266
	W797	F711	G616	L492	H399	N274
		M713	A616	L493	L400	R277
	V801	R714	L715	L494	E401	
	L802	D716	D717		I402	P281
	S808	D717	V718	K506	I403	
		V718	A719	L622	Y404	R292
	R815	A719		V512	E405	
	K818		D722	V626	H410	E296
			A627	S516		
	S830	Y726		T519	R413	V300
ASP		E727	V630	K520	I414	A301
LEU		A728		L521	A416	Q305
LYS		K729	D633			D306
ILE						

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	124.63Å 124.63Å 124.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (99.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.236 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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, MPD

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	0.42	0/6520	0.93	29/8818 (0.3%)
1	B	0.41	0/6520	0.92	26/8818 (0.3%)
All	All	0.41	0/13040	0.93	55/17636 (0.3%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	VAL	N-CA-C	8.25	119.66	108.11
1	B	565	VAL	N-CA-C	8.04	119.37	108.11
1	A	91	MET	N-CA-C	7.98	121.08	111.82
1	B	91	MET	N-CA-C	7.98	121.08	111.82
1	B	354	VAL	N-CA-C	7.63	117.68	110.74
1	A	354	VAL	N-CA-C	7.51	117.58	110.74
1	B	576	GLN	N-CA-C	-7.43	103.48	112.54
1	A	575	ARG	N-CA-C	7.22	121.62	111.52
1	B	575	ARG	N-CA-C	7.10	121.47	111.52
1	B	203	TYR	CB-CA-C	-6.56	109.02	116.63
1	A	576	GLN	N-CA-C	-6.49	104.63	112.54
1	A	206	VAL	N-CA-C	6.36	117.75	108.53
1	A	203	TYR	CB-CA-C	-6.35	109.26	116.63
1	B	650	VAL	N-CA-C	6.18	116.85	110.36
1	B	216	ILE	N-CA-C	6.13	117.67	108.96
1	A	64	VAL	N-CA-C	6.11	116.59	110.23
1	B	64	VAL	N-CA-C	6.07	116.55	110.23
1	B	454	GLY	N-CA-C	-5.92	103.53	112.60
1	A	650	VAL	N-CA-C	5.92	116.58	110.36
1	A	454	GLY	N-CA-C	-5.92	103.55	112.60
1	B	656	VAL	N-CA-C	5.84	116.62	110.72
1	A	418	PHE	CA-C-N	5.75	127.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	PHE	C-N-CA	5.75	127.02	119.84
1	A	166	PHE	N-CA-C	5.74	117.70	110.24
1	A	372	PHE	N-CA-C	5.71	118.98	110.52
1	A	216	ILE	N-CA-C	5.69	117.04	108.96
1	B	166	PHE	N-CA-C	5.64	117.57	110.24
1	B	418	PHE	CA-C-N	5.61	126.85	119.84
1	B	418	PHE	C-N-CA	5.61	126.85	119.84
1	B	372	PHE	N-CA-C	5.57	118.77	110.52
1	A	232	GLY	N-CA-C	-5.50	105.23	112.82
1	A	735	LEU	CA-C-N	5.43	125.07	119.05
1	A	735	LEU	C-N-CA	5.43	125.07	119.05
1	A	754	GLN	CA-C-N	5.38	126.56	119.84
1	A	754	GLN	C-N-CA	5.38	126.56	119.84
1	A	24	VAL	N-CA-C	5.35	115.55	110.42
1	B	475	GLU	CA-C-N	5.34	124.79	119.24
1	B	475	GLU	C-N-CA	5.34	124.79	119.24
1	B	754	GLN	CA-C-N	5.33	126.50	119.84
1	B	754	GLN	C-N-CA	5.33	126.50	119.84
1	B	333	VAL	N-CA-C	5.31	115.54	108.11
1	A	129	ALA	N-CA-C	-5.29	99.36	108.56
1	A	333	VAL	N-CA-C	5.23	115.43	108.11
1	A	675	GLY	N-CA-C	-5.23	106.16	112.48
1	B	76	ASP	N-CA-C	5.23	116.79	111.14
1	A	677	GLY	N-CA-C	-5.21	106.39	113.37
1	B	666	ILE	N-CA-C	5.20	120.15	109.34
1	B	232	GLY	N-CA-C	-5.19	105.66	112.82
1	A	684	ASN	N-CA-C	5.17	119.28	112.92
1	A	656	VAL	N-CA-C	5.12	115.89	110.72
1	B	735	LEU	CA-C-N	5.04	124.65	119.05
1	B	735	LEU	C-N-CA	5.04	124.65	119.05
1	A	676	THR	N-CA-C	-5.03	108.41	114.75
1	A	162	GLU	N-CA-C	-5.01	106.00	111.82
1	B	182	TRP	N-CA-C	5.01	118.49	112.38

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	6377	0	6372	157	0
1	B	6377	0	6372	170	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	18	0	0
4	B	30	0	18	0	0
5	A	8	0	14	1	0
5	B	8	0	14	0	0
6	A	174	0	0	7	0
6	B	159	0	0	12	0
All	All	13223	0	12852	325	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 13.

All (325) 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:96:GLN:HE21	1:A:105:GLN:HE22	1.11	0.98
1:B:96:GLN:HE21	1:B:105:GLN:HE22	1.09	0.98
1:A:168:GLN:HE21	1:A:647:ASN:H	1.21	0.87
1:B:168:GLN:HE21	1:B:647:ASN:H	1.22	0.87
1:B:81:ARG:NH1	1:B:310:ARG:HD3	1.94	0.81
1:A:81:ARG:NH1	1:A:310:ARG:HD3	1.94	0.81
1:B:33:ARG:HD2	6:B:2232:HOH:O	1.80	0.79
1:B:455:VAL:H	1:B:459:HIS:HD2	1.31	0.78
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.67	0.75
1:A:96:GLN:NE2	1:A:105:GLN:HE22	1.84	0.75
1:B:96:GLN:NE2	1:B:105:GLN:HE22	1.82	0.74
1:A:547:GLN:O	1:A:551:THR:HG23	1.89	0.73
1:A:455:VAL:H	1:A:459:HIS:HD2	1.34	0.73
1:B:692:MET:HG3	1:B:697:VAL:HG22	1.69	0.73
1:B:96:GLN:HE21	1:B:105:GLN:NE2	1.86	0.72
1:A:197:MET:HE3	1:A:224:LEU:HB2	1.72	0.72
1:B:197:MET:HE3	1:B:224:LEU:HB2	1.71	0.72
1:B:759:LYS:HB3	1:B:759:LYS:NZ	2.05	0.72
1:A:759:LYS:NZ	1:A:759:LYS:HB3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:HD22	1:B:277:ARG:HH11	1.40	0.70
1:B:547:GLN:O	1:B:551:THR:HG23	1.91	0.70
1:A:274:ASN:HD22	1:A:277:ARG:HH11	1.39	0.68
1:A:792:MET:O	1:A:794:PRO:HD3	1.94	0.68
1:B:792:MET:O	1:B:794:PRO:HD3	1.93	0.67
1:B:274:ASN:ND2	1:B:277:ARG:HH11	1.93	0.67
1:A:96:GLN:HE21	1:A:105:GLN:NE2	1.91	0.67
1:B:44:ASN:HD22	1:B:45:VAL:N	1.93	0.66
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.93	0.66
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.31	0.66
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.31	0.65
1:B:66:ARG:HD3	1:B:236:ASN:HA	1.79	0.65
1:A:44:ASN:HD22	1:A:45:VAL:N	1.94	0.64
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.77	0.64
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.78	0.63
1:A:433:GLU:HG3	1:A:437:LYS:HE3	1.80	0.63
1:A:66:ARG:HD3	1:A:236:ASN:HA	1.80	0.63
1:B:433:GLU:HG3	1:B:437:LYS:HE3	1.80	0.63
1:A:413:ARG:HA	1:A:413:ARG:HE	1.64	0.62
1:A:571:HIS:HD2	1:A:573:TYR:H	1.49	0.61
1:A:42:ASP:HB2	1:A:44:ASN:HD21	1.66	0.60
1:B:96:GLN:HB2	6:B:2289:HOH:O	2.00	0.60
1:B:727:GLU:HG2	1:B:729:LYS:HG2	1.83	0.60
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.36	0.60
1:B:571:HIS:HD2	1:B:573:TYR:H	1.48	0.60
1:B:630:VAL:O	1:B:636:VAL:HG21	2.02	0.60
1:B:413:ARG:HE	1:B:413:ARG:HA	1.65	0.60
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.84	0.59
1:B:211:THR:OG1	1:B:214:LYS:HE2	2.02	0.59
1:B:546:SER:O	1:B:550:GLU:HG2	2.02	0.59
1:B:732:TYR:CZ	1:B:739:LYS:HG3	2.37	0.59
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.85	0.59
1:B:42:ASP:HB2	1:B:44:ASN:HD21	1.68	0.59
1:A:727:GLU:HG2	1:A:729:LYS:HG2	1.83	0.59
1:B:494:LEU:C	1:B:494:LEU:HD23	2.28	0.58
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.85	0.58
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.85	0.58
1:B:28:LYS:HD2	1:B:115:LEU:HG	1.85	0.58
1:B:579:ASN:C	1:B:579:ASN:HD22	2.10	0.58
1:A:579:ASN:C	1:A:579:ASN:HD22	2.10	0.58
1:A:380:LEU:HD12	1:A:380:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:TYR:CE1	1:A:739:LYS:HA	2.39	0.58
1:A:546:SER:O	1:A:550:GLU:HG2	2.04	0.57
1:B:605:ILE:O	1:B:644:PHE:HA	2.04	0.57
1:A:29:LYS:HE2	1:A:33:ARG:HH21	1.70	0.57
1:A:630:VAL:O	1:A:636:VAL:HG21	2.04	0.57
1:A:28:LYS:HD2	1:A:115:LEU:HG	1.85	0.57
1:B:380:LEU:HD12	1:B:380:LEU:H	1.70	0.57
1:B:732:TYR:CE1	1:B:739:LYS:HA	2.40	0.56
1:A:386:ARG:HA	1:A:439:ILE:O	2.05	0.56
1:A:494:LEU:HD23	1:A:494:LEU:C	2.30	0.56
1:B:386:ARG:HA	1:B:439:ILE:O	2.04	0.56
1:A:93:ARG:O	1:A:490:ARG:NH2	2.38	0.56
1:B:207:GLU:HG2	1:B:209:THR:HG23	1.86	0.56
1:A:770:ARG:HG2	6:A:2155:HOH:O	2.05	0.56
1:B:29:LYS:HE2	1:B:33:ARG:HH21	1.71	0.56
1:A:633:ASP:O	1:A:636:VAL:HG22	2.06	0.56
1:A:525:LEU:HD23	1:A:802:LEU:HD23	1.87	0.55
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.87	0.55
1:B:45:VAL:HG12	1:B:45:VAL:O	2.05	0.55
1:B:361:TRP:CH2	1:B:405:GLU:HB3	2.42	0.55
1:B:633:ASP:O	1:B:636:VAL:HG22	2.05	0.55
1:B:93:ARG:O	1:B:490:ARG:NH2	2.39	0.55
1:B:597:LEU:O	1:B:597:LEU:HD12	2.07	0.55
1:A:45:VAL:HG12	1:A:45:VAL:O	2.06	0.55
1:A:597:LEU:HD12	1:A:597:LEU:O	2.07	0.55
1:A:571:HIS:CD2	1:A:573:TYR:H	2.24	0.55
1:A:605:ILE:O	1:A:644:PHE:HA	2.08	0.54
1:A:488:PRO:O	1:A:492:LEU:HB3	2.06	0.54
1:A:42:ASP:HB2	1:A:44:ASN:ND2	2.22	0.54
1:B:301:ALA:O	1:B:305:GLN:HG3	2.08	0.54
1:B:247:ARG:HD2	6:B:2116:HOH:O	2.07	0.53
1:A:713:MET:HB3	1:A:717:ASP:HB2	1.90	0.53
1:B:44:ASN:ND2	1:B:45:VAL:HG23	2.23	0.53
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.90	0.53
1:A:386:ARG:HH21	1:A:438:ARG:HD2	1.73	0.53
1:B:571:HIS:CD2	1:B:573:TYR:H	2.24	0.53
1:B:488:PRO:O	1:B:492:LEU:HB3	2.08	0.53
1:A:361:TRP:CH2	1:A:405:GLU:HB3	2.44	0.53
1:A:490:ARG:NH1	6:A:2231:HOH:O	2.41	0.53
1:B:235:ASN:O	1:B:236:ASN:HB2	2.08	0.53
1:B:386:ARG:HH21	1:B:438:ARG:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ALA:O	1:A:305:GLN:HG3	2.10	0.52
1:A:557:ILE:O	1:A:559:PRO:HD3	2.09	0.52
1:A:565:VAL:HG22	1:A:604:ILE:HB	1.91	0.52
1:A:689:ILE:HG23	1:A:689:ILE:O	2.08	0.52
1:B:410:HIS:HE1	1:B:428:MET:O	1.92	0.52
1:B:525:LEU:HD23	1:B:802:LEU:HD23	1.90	0.52
1:A:235:ASN:O	1:A:236:ASN:HB2	2.10	0.52
1:A:455:VAL:H	1:A:459:HIS:CD2	2.23	0.52
1:A:545:PHE:O	1:A:548:PHE:HB3	2.10	0.52
1:A:423:ASP:O	1:A:427:ARG:HB2	2.09	0.52
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.93	0.52
1:B:575:ARG:HD2	1:B:666:ILE:O	2.09	0.51
1:B:106:ASN:HB3	6:B:2162:HOH:O	2.08	0.51
1:B:708:LEU:HG	6:B:2114:HOH:O	2.09	0.51
1:A:693:ASP:O	1:A:696:ASN:HB2	2.11	0.51
1:A:764:MET:HE1	1:A:765:LEU:HD13	1.92	0.51
1:B:42:ASP:HB2	1:B:44:ASN:ND2	2.25	0.51
1:A:490:ARG:NH1	6:A:2139:HOH:O	2.44	0.51
1:B:80:LYS:HE2	1:B:334:ALA:HB2	1.93	0.51
1:B:181:ASP:OD2	1:B:184:ARG:HB2	2.11	0.51
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.93	0.51
1:B:587:TYR:O	1:B:591:LYS:HG2	2.11	0.51
1:B:423:ASP:O	1:B:427:ARG:HB2	2.11	0.50
1:A:410:HIS:HE1	1:A:428:MET:O	1.95	0.50
1:A:737:GLU:O	1:A:741:VAL:HG23	2.11	0.50
1:A:795:LYS:HB2	6:A:2180:HOH:O	2.10	0.50
1:B:262:TYR:O	1:B:266:VAL:HG23	2.11	0.50
1:B:693:ASP:O	1:B:696:ASN:HB2	2.11	0.50
1:B:759:LYS:HB3	1:B:759:LYS:HZ2	1.75	0.50
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.94	0.50
1:B:341:HIS:HB2	1:B:342:PRO:HD3	1.93	0.50
1:B:557:ILE:O	1:B:559:PRO:HD3	2.11	0.50
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.93	0.49
1:A:44:ASN:ND2	1:A:45:VAL:HG23	2.26	0.49
1:B:455:VAL:H	1:B:459:HIS:CD2	2.21	0.49
1:B:545:PHE:O	1:B:548:PHE:HB3	2.12	0.49
1:A:102:LEU:O	1:A:104:LEU:HD13	2.12	0.49
1:A:469:LYS:HG2	1:A:473:GLU:OE2	2.11	0.49
1:A:587:TYR:O	1:A:591:LYS:HG2	2.13	0.49
1:B:434:GLU:CD	1:B:434:GLU:H	2.21	0.49
1:B:174:TRP:CE2	1:B:621:LYS:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:C	1:B:417:LEU:H	2.20	0.49
1:B:689:ILE:O	1:B:689:ILE:HG23	2.11	0.49
1:B:24:VAL:HB	6:B:2301:HOH:O	2.13	0.49
1:A:80:LYS:HE2	1:A:334:ALA:HB2	1.94	0.49
1:B:732:TYR:CE1	1:B:739:LYS:HG3	2.48	0.49
1:A:174:TRP:CE2	1:A:621:LYS:HG3	2.48	0.49
1:A:422:VAL:HG23	1:A:423:ASP:N	2.27	0.49
1:B:422:VAL:HG23	1:B:423:ASP:N	2.28	0.49
1:A:415:VAL:C	1:A:417:LEU:H	2.21	0.48
1:A:446:ILE:HD11	1:A:468:PHE:CD2	2.48	0.48
1:A:823:ASN:ND2	6:A:2241:HOH:O	2.46	0.48
1:B:764:MET:HE1	1:B:765:LEU:HD13	1.95	0.48
1:A:44:ASN:HD22	1:A:44:ASN:C	2.19	0.48
1:A:181:ASP:OD2	1:A:184:ARG:HB2	2.13	0.48
1:B:66:ARG:CD	1:B:236:ASN:HA	2.43	0.48
1:A:562:MET:HE1	1:A:787:VAL:HG12	1.95	0.48
1:A:566:GLN:HB2	1:A:664:GLU:HG3	1.96	0.48
1:B:566:GLN:HB2	1:B:664:GLU:HG3	1.94	0.48
1:B:735:LEU:HD22	1:B:778:GLU:HG3	1.96	0.48
1:A:133:ASN:OD1	1:A:281:PRO:HA	2.14	0.48
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.95	0.48
1:A:715:ILE:HG23	1:A:716:ASP:N	2.28	0.48
1:B:133:ASN:OD1	1:B:281:PRO:HA	2.13	0.48
1:A:399:HIS:O	1:A:403:ILE:HG13	2.14	0.48
1:B:44:ASN:HD22	1:B:44:ASN:C	2.19	0.48
1:B:728:ALA:HB1	1:B:774:PHE:CD1	2.49	0.48
1:B:737:GLU:O	1:B:741:VAL:HG23	2.13	0.48
1:A:262:TYR:O	1:A:266:VAL:HG23	2.13	0.48
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.48	0.48
1:B:446:ILE:HD11	1:B:468:PHE:CD2	2.49	0.48
1:B:729:LYS:HG3	1:B:730:GLU:N	2.29	0.48
1:A:735:LEU:HD22	1:A:778:GLU:HG3	1.96	0.48
1:B:185:TYR:HA	6:B:2144:HOH:O	2.14	0.48
1:A:66:ARG:CD	1:A:236:ASN:HA	2.42	0.48
1:A:398:ARG:O	1:A:402:ILE:HG13	2.14	0.47
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.44	0.47
1:B:740:LEU:O	1:B:744:GLN:HG3	2.14	0.47
1:A:759:LYS:HB3	1:A:759:LYS:HZ3	1.78	0.47
1:B:617:LYS:HD3	6:B:2224:HOH:O	2.14	0.47
1:A:729:LYS:HG3	1:A:730:GLU:N	2.29	0.47
1:A:575:ARG:HD2	1:A:666:ILE:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:MET:HE1	1:B:787:VAL:HG12	1.96	0.47
1:B:206:VAL:HG11	1:B:401:GLU:OE2	2.14	0.47
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.97	0.47
1:A:434:GLU:H	1:A:434:GLU:CD	2.22	0.47
1:B:417:LEU:C	1:B:419:PRO:HD3	2.40	0.47
1:B:418:PHE:N	1:B:419:PRO:HD3	2.30	0.47
1:B:469:LYS:HG2	1:B:473:GLU:OE2	2.14	0.47
1:B:636:VAL:O	1:B:639:LYS:HB2	2.15	0.47
1:B:29:LYS:HE2	1:B:33:ARG:NH2	2.29	0.47
1:B:710:ILE:HG22	1:B:711:PHE:N	2.30	0.47
1:A:29:LYS:HE2	1:A:33:ARG:NH2	2.29	0.46
1:B:157:TYR:HD2	1:B:244:TRP:HE1	1.64	0.46
1:B:168:GLN:NE2	1:B:647:ASN:H	2.03	0.46
1:B:792:MET:C	1:B:794:PRO:HD3	2.39	0.46
1:A:28:LYS:HG2	1:A:111:ALA:HB1	1.96	0.46
1:A:636:VAL:O	1:A:639:LYS:HB2	2.15	0.46
1:B:29:LYS:HE2	1:B:29:LYS:HB3	1.70	0.46
1:B:193:ARG:HB2	1:B:225:PRO:HG2	1.97	0.46
1:B:746:ASP:HB2	1:B:762:ILE:HG13	1.96	0.46
1:A:728:ALA:HB1	1:A:774:PHE:CD1	2.51	0.46
1:B:431:ILE:HG22	1:B:433:GLU:OE1	2.14	0.46
1:A:746:ASP:HB2	1:A:762:ILE:HG13	1.97	0.46
1:A:522:HIS:O	1:A:525:LEU:HG	2.16	0.46
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.55	0.46
1:B:715:ILE:HG23	1:B:716:ASP:N	2.31	0.46
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.96	0.46
1:B:28:LYS:HG2	1:B:111:ALA:HB1	1.97	0.46
1:A:126:GLU:HB3	6:A:2147:HOH:O	2.16	0.46
1:B:428:MET:HE1	1:B:474:LEU:HD12	1.98	0.46
1:B:627:ALA:HA	1:B:642:VAL:HB	1.98	0.46
1:A:417:LEU:C	1:A:419:PRO:HD3	2.41	0.45
1:A:418:PHE:N	1:A:419:PRO:HD3	2.30	0.45
1:A:29:LYS:HE2	1:A:29:LYS:HB3	1.74	0.45
1:A:690:GLY:O	1:A:710:ILE:HA	2.16	0.45
1:A:181:ASP:OD2	1:A:184:ARG:NE	2.49	0.45
1:A:792:MET:C	1:A:794:PRO:HD3	2.41	0.45
1:B:399:HIS:O	1:B:403:ILE:HG13	2.16	0.45
1:A:428:MET:HE1	1:A:474:LEU:HD12	1.97	0.45
1:A:168:GLN:NE2	6:A:2007:HOH:O	2.49	0.45
1:A:579:ASN:C	1:A:579:ASN:ND2	2.75	0.45
1:A:721:LEU:HD23	1:A:772:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASP:OD2	1:B:184:ARG:NE	2.49	0.45
1:A:431:ILE:HG22	1:A:433:GLU:OE1	2.17	0.44
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.57	0.44
1:A:281:PRO:HG3	1:B:262:TYR:CE2	2.52	0.44
1:B:133:ASN:HB2	6:B:2025:HOH:O	2.16	0.44
1:B:150:LEU:HD21	1:B:818:LYS:HG3	1.99	0.44
1:B:682:MET:HG2	1:B:808:SER:HB3	1.99	0.44
1:A:136:LEU:HD11	1:A:338:ASN:ND2	2.32	0.44
1:A:168:GLN:NE2	1:A:647:ASN:H	2.02	0.44
1:A:170:ILE:CG1	1:A:646:GLU:HG2	2.47	0.44
1:A:740:LEU:O	1:A:744:GLN:HG3	2.17	0.44
1:B:98:THR:O	1:B:102:LEU:HB2	2.18	0.44
1:B:797:TRP:O	1:B:801:VAL:HG23	2.17	0.44
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.64	0.44
1:A:719:ALA:O	1:A:722:ASP:HB2	2.17	0.44
1:B:693:ASP:O	1:B:694:GLY:C	2.61	0.44
1:B:690:GLY:O	1:B:710:ILE:HA	2.18	0.44
1:A:627:ALA:HA	1:A:642:VAL:HB	2.00	0.44
1:A:571:HIS:CD2	1:A:572:GLU:N	2.86	0.44
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.85	0.44
1:A:759:LYS:HB3	1:A:759:LYS:HZ2	1.79	0.44
1:B:233:TYR:CE2	1:B:512:VAL:HG11	2.53	0.44
1:B:398:ARG:O	1:B:402:ILE:HG13	2.18	0.44
1:B:522:HIS:O	1:B:525:LEU:HG	2.17	0.44
1:B:553:TYR:CD1	1:B:553:TYR:N	2.86	0.44
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.43	0.43
1:B:136:LEU:HD11	1:B:338:ASN:ND2	2.33	0.43
1:A:193:ARG:NH1	5:A:1901:MPD:HM2	2.33	0.43
1:B:528:ASP:O	1:B:532:ARG:HD3	2.19	0.43
1:A:128:ASP:OD2	1:A:651:SER:HB3	2.18	0.43
1:B:622:LEU:HA	1:B:758:PHE:CZ	2.53	0.43
1:A:387:TRP:HA	1:A:388:PRO:HD3	1.89	0.43
1:A:553:TYR:CD1	1:A:553:TYR:N	2.86	0.43
1:B:450:HIS:HE1	6:B:2193:HOH:O	2.00	0.43
1:B:421:ASP:CG	1:B:424:ARG:HB2	2.43	0.43
1:B:719:ALA:O	1:B:722:ASP:HB2	2.18	0.43
1:B:579:ASN:C	1:B:579:ASN:ND2	2.74	0.43
1:B:36:HIS:O	1:B:40:VAL:HA	2.19	0.43
1:B:128:ASP:OD2	1:B:651:SER:HB3	2.19	0.43
1:B:571:HIS:CD2	1:B:572:GLU:N	2.86	0.43
1:B:726:TYR:OH	1:B:774:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LEU:HA	1:A:758:PHE:CZ	2.54	0.43
1:B:735:LEU:HA	1:B:736:PRO:HD2	1.86	0.43
1:B:815:ARG:HD2	1:B:815:ARG:C	2.44	0.43
1:A:636:VAL:HG23	1:A:637:GLY:N	2.33	0.42
1:B:138:ARG:HA	1:B:138:ARG:HD2	1.90	0.42
1:A:568:LYS:O	1:A:607:GLY:HA3	2.19	0.42
1:A:36:HIS:O	1:A:40:VAL:HA	2.19	0.42
1:A:710:ILE:HG22	1:A:711:PHE:N	2.33	0.42
1:B:615:MET:HE2	1:B:764:MET:HE2	2.00	0.42
1:A:138:ARG:HA	1:A:138:ARG:HD2	1.92	0.42
1:A:615:MET:HE2	1:A:764:MET:HE2	2.01	0.42
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.20	0.42
1:A:622:LEU:O	1:A:626:VAL:HG23	2.19	0.42
1:A:682:MET:HG2	1:A:808:SER:HB3	2.01	0.42
1:A:793:ASN:ND2	1:A:796:ALA:HB2	2.35	0.42
1:B:636:VAL:HG23	1:B:637:GLY:N	2.33	0.42
1:A:374:TYR:O	1:A:452:VAL:HA	2.19	0.42
1:A:815:ARG:C	1:A:815:ARG:HD2	2.44	0.42
1:B:381:PRO:HA	1:B:384:LEU:HG	2.02	0.42
1:A:797:TRP:O	1:A:801:VAL:HG23	2.20	0.41
1:B:420:LYS:O	1:B:422:VAL:N	2.53	0.41
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.87	0.41
1:A:693:ASP:O	1:A:694:GLY:C	2.62	0.41
1:B:205:LYS:HE3	1:B:217:ASP:HB2	2.02	0.41
1:B:23:ASN:O	1:B:24:VAL:C	2.63	0.41
1:B:374:TYR:O	1:B:452:VAL:HA	2.20	0.41
1:B:711:PHE:HA	6:B:2251:HOH:O	2.19	0.41
1:A:112:ILE:HG23	1:A:117:LEU:HB2	2.02	0.41
1:A:150:LEU:HD21	1:A:818:LYS:HG3	2.02	0.41
1:A:144:LEU:HB3	1:A:230:VAL:HG11	2.02	0.41
1:A:348:GLU:O	1:A:352:ILE:HG13	2.20	0.41
1:B:157:TYR:OH	1:B:306:ASP:OD2	2.35	0.41
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.55	0.41
1:B:144:LEU:HB3	1:B:230:VAL:HG11	2.02	0.41
1:A:751:SER:N	1:A:752:PRO:HD3	2.36	0.41
1:A:42:ASP:CB	1:A:44:ASN:ND2	2.84	0.41
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.56	0.41
1:B:112:ILE:HG23	1:B:117:LEU:HB2	2.02	0.41
1:A:420:LYS:O	1:A:422:VAL:N	2.54	0.41
1:A:726:TYR:OH	1:A:774:PHE:HB2	2.21	0.41
1:B:292:ARG:O	1:B:296:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:HG23	1:B:459:HIS:N	2.36	0.41
1:B:793:ASN:ND2	1:B:796:ALA:HB2	2.35	0.41
1:A:43:ARG:HD2	1:A:43:ARG:HA	1.92	0.41
1:A:458:ILE:HG23	1:A:459:HIS:N	2.35	0.41
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.54	0.41
1:B:168:GLN:NE2	6:B:2237:HOH:O	2.46	0.41
1:B:566:GLN:HG3	1:B:664:GLU:HB2	2.04	0.40
1:B:571:HIS:HD2	1:B:572:GLU:N	2.19	0.40
1:B:622:LEU:O	1:B:626:VAL:HG23	2.21	0.40
1:B:698:GLU:O	1:B:702:GLU:HG2	2.21	0.40
1:B:751:SER:N	1:B:752:PRO:HD3	2.36	0.40
1:B:300:VAL:HG13	1:B:345:ALA:HA	2.03	0.40
1:B:521:LEU:HB3	1:B:802:LEU:HD11	2.03	0.40
1:A:262:TYR:CE2	1:B:281:PRO:HG3	2.56	0.40
1:A:433:GLU:HA	1:A:437:LYS:HG2	2.04	0.40
1:B:433:GLU:HA	1:B:437:LYS:HG2	2.04	0.40
1:A:571:HIS:HD2	1:A:572:GLU:N	2.18	0.40
1:B:45:VAL:O	1:B:45:VAL:CG1	2.69	0.40
1:B:516:SER:O	1:B:519:THR:HG23	2.22	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	780/847 (92%)	731 (94%)	48 (6%)	1 (0%)	48	64
1	B	780/847 (92%)	730 (94%)	50 (6%)	0	100	100
All	All	1560/1694 (92%)	1461 (94%)	98 (6%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/740 (32%)	233 (97%)	7 (3%)	37	60
1	B	466/740 (63%)	448 (96%)	18 (4%)	28	48
All	All	706/1480 (48%)	681 (96%)	25 (4%)	32	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
1	A	426	ARG
1	A	433	GLU
1	A	551	THR
1	A	622	LEU
1	A	683	LEU
1	A	759	LYS
1	B	39	LEU
1	B	44	ASN
1	B	102	LEU
1	B	104	LEU
1	B	219	GLN
1	B	243	LEU
1	B	337	LEU
1	B	405	GLU
1	B	426	ARG
1	B	433	GLU
1	B	592	LYS
1	B	622	LEU
1	B	645	LEU
1	B	652	LEU
1	B	683	LEU
1	B	759	LYS

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Mol	Chain	Res	Type
1	B	765	LEU
1	B	770	ARG

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

Mol	Chain	Res	Type
1	A	369	GLN
1	A	410	HIS
1	A	453	ASN
1	A	459	HIS
1	A	566	GLN
1	A	804	ASN
1	B	44	ASN
1	B	62	HIS
1	B	105	GLN
1	B	114	GLN
1	B	236	ASN
1	B	239	ASN
1	B	305	GLN
1	B	369	GLN
1	B	410	HIS
1	B	450	HIS
1	B	453	ASN
1	B	459	HIS
1	B	789	GLN
1	B	793	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	700	A	862	-	31,33,33	2.80	15 (48%)	44,47,47	1.98	11 (25%)
2	NBG	A	861	-	15,15,15	1.39	3 (20%)	21,21,21	1.18	1 (4%)
5	MPD	B	1902	-	7,7,7	0.77	0	9,10,10	0.77	0
4	700	B	1862	-	31,33,33	2.84	17 (54%)	44,47,47	1.86	11 (25%)
3	PLP	B	1860	1	15,15,16	1.88	2 (13%)	21,22,23	1.40	4 (19%)
2	NBG	B	1861	-	15,15,15	1.62	3 (20%)	21,21,21	1.34	2 (9%)
5	MPD	A	1901	-	7,7,7	0.51	0	9,10,10	0.79	0
3	PLP	A	860	1	15,15,16	1.54	1 (6%)	21,22,23	1.46	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	700	A	862	-	-	0/22/32/32	0/4/4/4
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
5	MPD	B	1902	-	1/1/2/2	1/5/5/5	-
4	700	B	1862	-	-	1/22/32/32	0/4/4/4
3	PLP	B	1860	1	-	2/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
5	MPD	A	1901	-	1/1/2/2	3/5/5/5	-
3	PLP	A	860	1	-	1/6/6/8	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	862	700	C7-C8	9.72	1.52	1.37
4	B	1862	700	C7-C8	9.50	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C4A-C4	-5.77	1.40	1.51
4	A	862	700	C8-N2	-5.70	1.30	1.38
4	B	1862	700	C8-N2	-5.15	1.31	1.38
4	B	1862	700	C17-C18	-5.11	1.43	1.53
3	A	860	PLP	C4A-C4	-4.70	1.42	1.51
4	A	862	700	C17-C18	-4.61	1.44	1.53
2	B	1861	NBG	C2-C1	4.09	1.57	1.53
4	B	1862	700	C3-C4	3.39	1.44	1.38
4	A	862	700	C5-C4	3.38	1.43	1.38
2	A	861	NBG	C2-C1	3.37	1.56	1.53
4	B	1862	700	C5-C4	2.79	1.42	1.38
4	B	1862	700	C3-C2	2.75	1.43	1.38
4	B	1862	700	C12-C11	2.63	1.44	1.38
4	B	1862	700	C13-C12	2.63	1.43	1.38
2	B	1861	NBG	C1-N1	2.61	1.46	1.43
4	A	862	700	C12-C11	2.61	1.44	1.38
4	A	862	700	C3-C4	2.55	1.42	1.38
4	A	862	700	C15-C16	2.45	1.43	1.38
4	A	862	700	C6-C7	2.43	1.51	1.44
4	A	862	700	C3-C2	2.42	1.42	1.38
4	B	1862	700	C16-C11	2.39	1.43	1.38
2	B	1861	NBG	C4-C5	2.31	1.57	1.53
4	B	1862	700	C9-N1	2.29	1.39	1.34
2	A	861	NBG	C3-C2	2.26	1.58	1.52
4	B	1862	700	C15-C16	2.26	1.42	1.38
4	B	1862	700	O4-C21	-2.20	1.23	1.30
4	B	1862	700	C10-C17	2.20	1.59	1.54
4	A	862	700	C13-C12	2.19	1.42	1.38
3	B	1860	PLP	C3-C2	-2.19	1.38	1.41
4	B	1862	700	C20-C21	2.16	1.55	1.51
4	B	1862	700	C10-C11	2.11	1.56	1.51
4	A	862	700	C15-C14	2.11	1.42	1.38
2	A	861	NBG	C1-N1	2.10	1.46	1.43
4	B	1862	700	C2-C1	2.08	1.43	1.39
4	A	862	700	C2-C1	2.07	1.43	1.39
4	A	862	700	C16-C11	2.06	1.43	1.38
4	B	1862	700	C6-C7	2.03	1.50	1.44
4	A	862	700	O4-C21	-2.02	1.24	1.30
4	A	862	700	C10-C17	2.00	1.58	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	862	700	C8-C9-N1	4.75	123.20	116.86
4	A	862	700	O1-C9-C8	-4.42	115.39	121.09
2	B	1861	NBG	C5-O5-C1	4.30	118.44	112.47
4	B	1862	700	C8-C9-N1	4.27	122.56	116.86
4	A	862	700	C1-C6-C7	-4.23	103.33	106.80
4	A	862	700	C1-N2-C8	4.16	113.47	109.01
4	B	1862	700	C5-C6-C1	4.07	121.65	119.13
4	B	1862	700	O1-C9-C8	-4.06	115.86	121.09
2	A	861	NBG	C5-O5-C1	3.86	117.83	112.47
4	B	1862	700	C1-C6-C7	-3.85	103.65	106.80
4	B	1862	700	C1-N2-C8	3.73	113.02	109.01
4	A	862	700	C6-C1-N2	3.66	111.46	107.65
4	A	862	700	C5-C6-C1	3.39	121.23	119.13
4	B	1862	700	C6-C1-N2	3.30	111.09	107.65
3	A	860	PLP	O3P-P-O4P	-3.13	98.51	106.67
4	A	862	700	C6-C7-C8	-3.11	104.63	107.41
4	A	862	700	O3-C21-C20	-3.09	114.66	122.86
4	A	862	700	O4-C21-O3	3.02	130.92	124.08
4	B	1862	700	O3-C21-C20	-2.85	115.31	122.86
4	B	1862	700	C6-C7-C8	-2.72	104.98	107.41
3	A	860	PLP	O3P-P-O2P	2.58	117.49	107.80
4	B	1862	700	O4-C21-O3	2.56	129.89	124.08
3	B	1860	PLP	O4P-P-O1P	-2.41	99.92	106.44
4	B	1862	700	C6-C5-C4	-2.40	117.52	120.40
3	A	860	PLP	C6-C5-C4	2.38	120.05	118.10
3	B	1860	PLP	C2A-C2-C3	2.25	123.44	120.80
4	A	862	700	C6-C5-C4	-2.25	117.70	120.40
3	A	860	PLP	C2A-C2-C3	2.24	123.42	120.80
3	B	1860	PLP	C6-C5-C4	2.22	119.92	118.10
3	B	1860	PLP	O2P-P-O4P	-2.21	100.91	106.67
4	B	1862	700	C19-C20-C21	2.16	121.50	116.40
2	B	1861	NBG	C2-C1-N1	-2.09	108.55	111.25
3	A	860	PLP	O4P-C5A-C5	-2.07	105.48	109.36
4	A	862	700	C7-C8-N2	-2.07	107.10	109.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1901	MPD	C4
5	B	1902	MPD	C4

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	860	PLP	C4-C5-C5A-O4P
3	B	1860	PLP	C5A-O4P-P-O1P
5	A	1901	MPD	C2-C3-C4-O4
5	A	1901	MPD	C2-C3-C4-C5
5	B	1902	MPD	C2-C3-C4-C5
4	B	1862	700	C22-C20-C21-O3
3	B	1860	PLP	C5A-O4P-P-O2P
5	A	1901	MPD	CM-C2-C3-C4

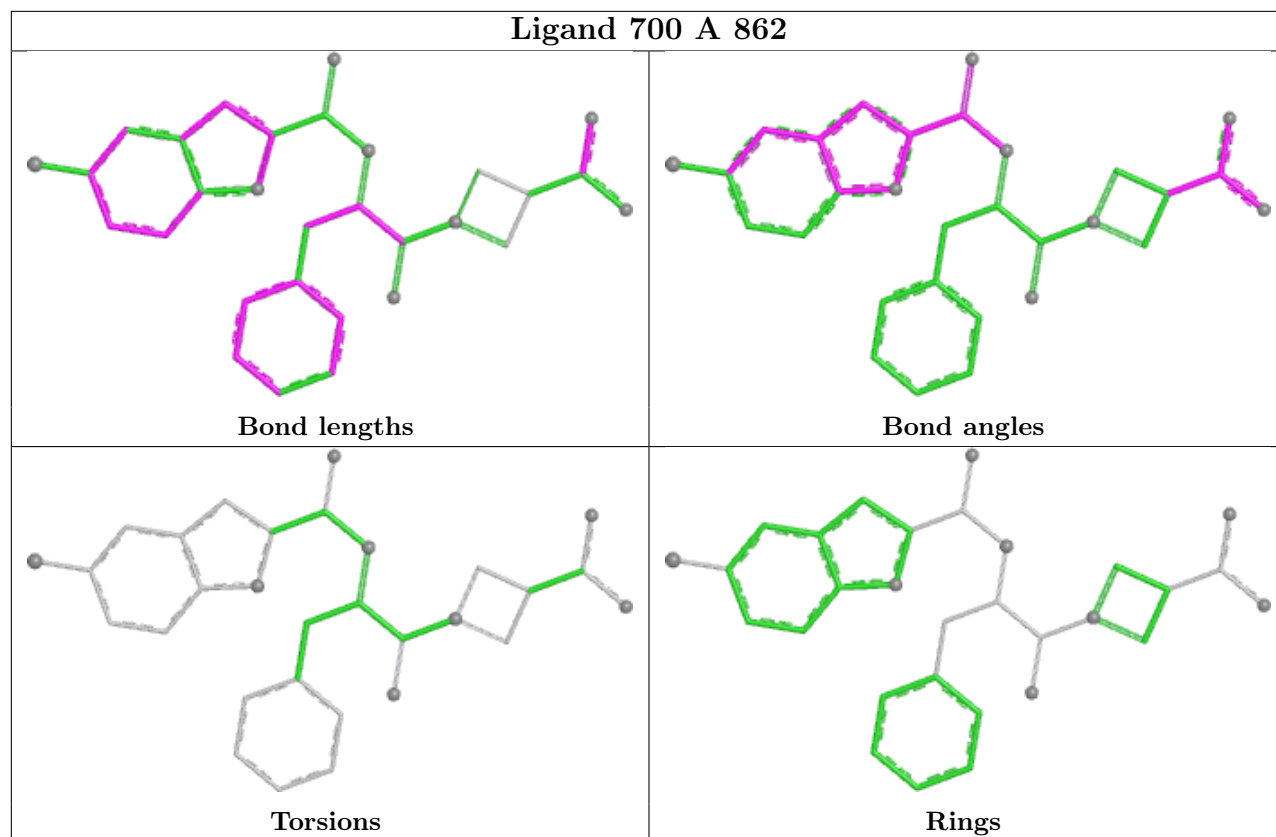
There are no ring outliers.

1 monomer is involved in 1 short contact:

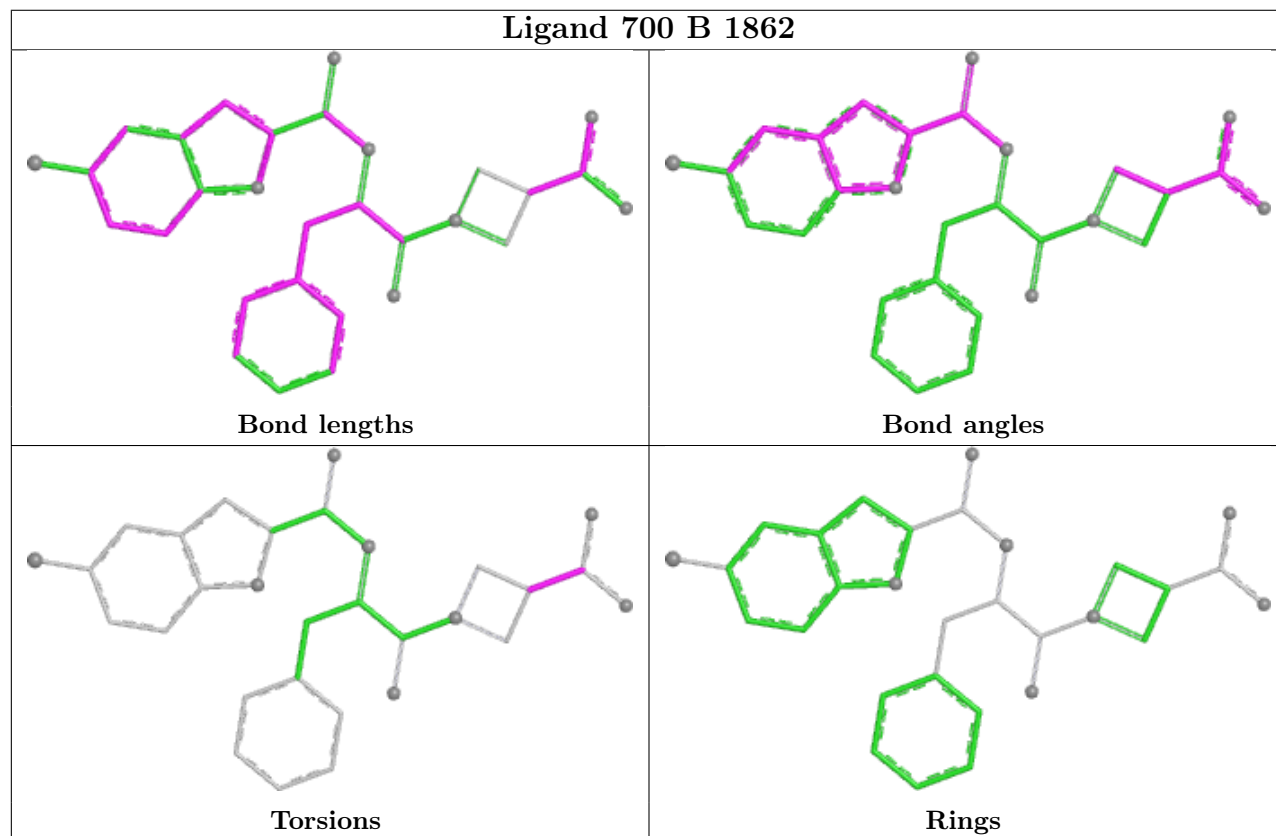
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1901	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 700 A 862



Ligand 700 B 1862



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.