



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 11:16 AM EDT

PDB ID : 1L5R  
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.; Myszka, 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

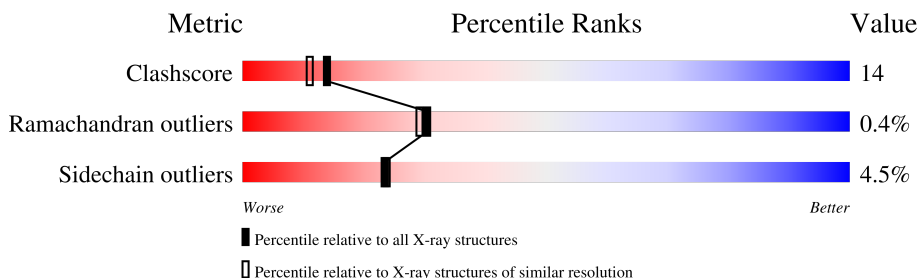
# 1 Overall quality at a glance

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	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (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  $\geq 3$ , 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](#)

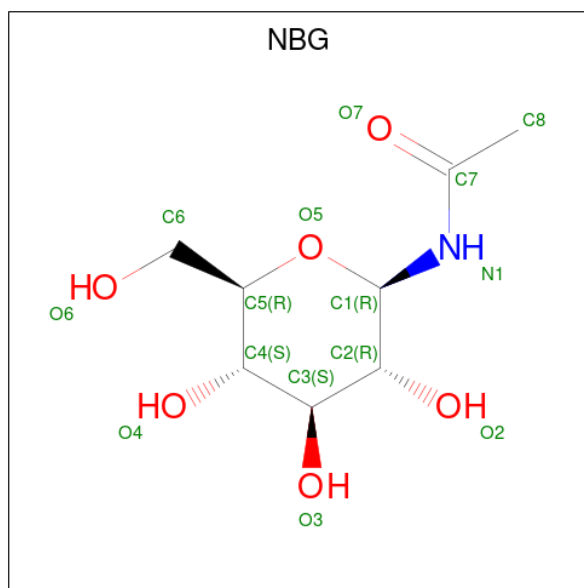
There are 7 unique types of molecules in this entry. The entry contains 13497 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: NBG) (formula:  $C_8H_{15}NO_6$ ).



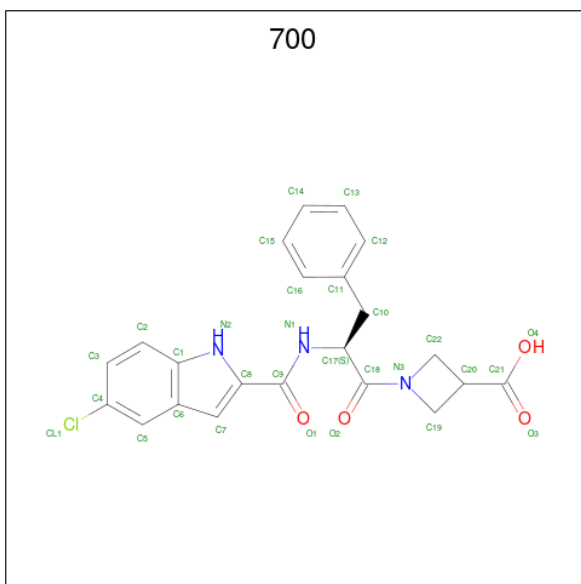
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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



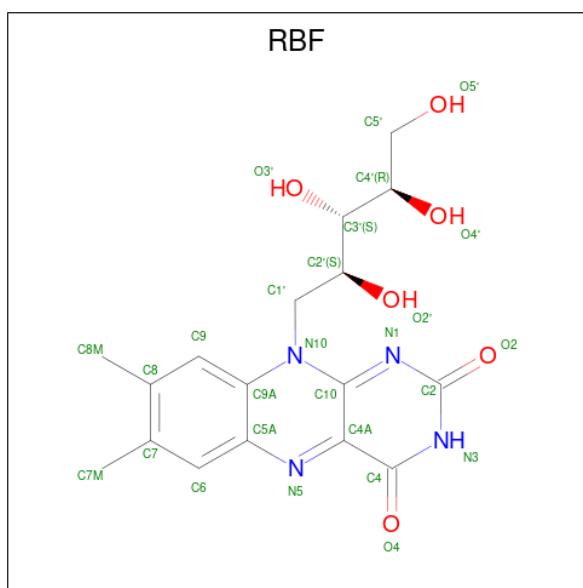
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is [5-CHLORO-1H-INDOL-2-CARBONYL-PHENYLALANINYL]-AZETIDINE-3-CARBOXYLIC ACID (three-letter code: 700) (formula: C<sub>22</sub>H<sub>20</sub>ClN<sub>3</sub>O<sub>4</sub>).



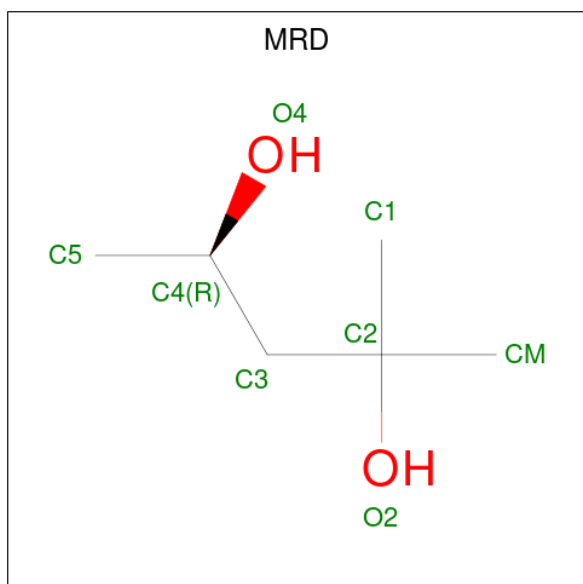
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is RIBOFLAVIN (three-letter code: 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 (three-letter code: 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.

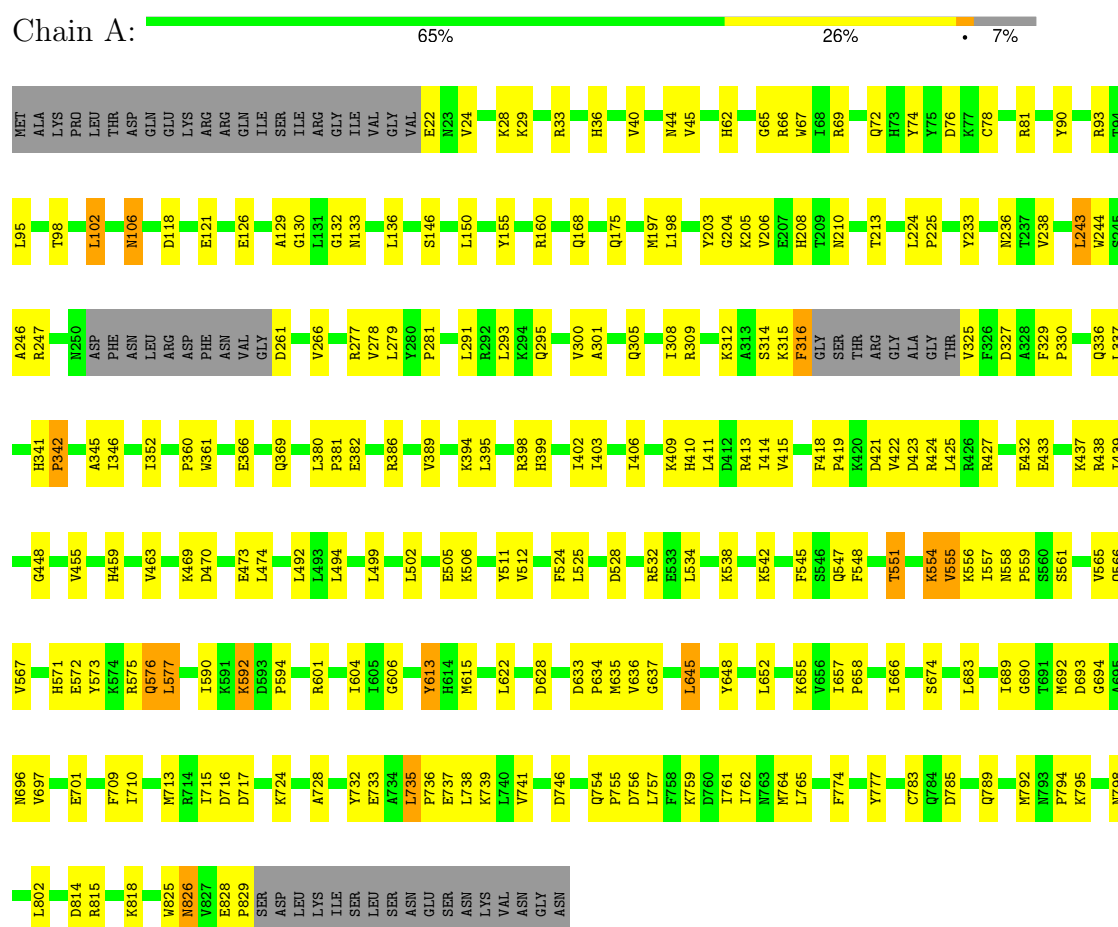
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	307	Total 307	O 307	0	0
7	B	240	Total 240	O 240	0	0

### 3 Residue-property plots

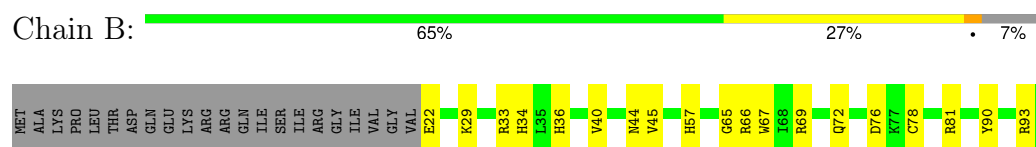
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: glycogen phosphorylase, liver form



D785	D786	Q789	M792	M793	P794	L802	D814	R815	K818	W825	N826	V827	E828	S830	ASP	LEU	LYS	ILE	SER	LEU	SER	ASN	GLU	SER	ASN	LYS	VAL	ASN	GLY	ASN	L102																			
T691	M692	D693	G694	A695	M696	V697	E701	L708	F709	L710	M713	R714	I715	D716	D717	K724	A728	Y732	E733	A734	L735	F736	E737	L738	K739	L740	V741	D746	P752	K753	Q754	P755	D756	L757	F758	K759	D760	I761	I762	M763	M764	L765	D769	F774	Y777	C783	Q784			
V565	Q566	V567	H571	E572	Y573	K574	R575	Q576	L577	K592	D593	P594	V599	P600	I604	L605	G606	Y613	H614	M615	M618	L622	D628	D633	P634	M635	V636	G637	L645	E646	N647	Y648	L652	K655	Q656	I657	P658	I666	S674	L683	I689	G690								
C445	F329	P330	Q336	L337	H341	P342	A345	I346	I352	W361	Y374	E382	R386	V389	K394	H399	I402	I403	I406	K409	H410	L411	D412	R413	I414	V415	F418	P419	K420	D421	V422	D423	R424	L425	R426	R427	E432	E433	K437	R438	I439	C445								
T237	V238	L243	W244	S245	A246	R247	N250	ASP	PHE	ASN	LEU	ASP	PHE	ASN	VAL	GLY	D261	V266	E273	R277	V278	P281	N282	D283	N284	F285	V300	A301	A302	T303	L304	Q305	T308	R309	R310	F311	K312	A313	S314	K315	F316	GLY	SER	THR	ARG	GLY	ALA	GLY	THR	V237
N106	E110	Y113	D118	E121	E124	E126	A129	M133	G134	G135	L136	S146	L150	Y155	G156	Y157	R160	Q168	K169	I170	Q175	S192	M197	L198	Y203	G204	K205	H208	T213	I216	L224	P225	Y233	N236																



## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	35.0	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: PLP, MRD, 700, RBF, NBG

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	0.44	0/6561	0.65	1/8873 (0.0%)
1	B	0.43	0/6567	0.65	1/8881 (0.0%)
All	All	0.43	0/13128	0.65	2/17754 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ALA	N-CA-C	-5.82	95.29	111.00
1	A	129	ALA	N-CA-C	-5.38	96.47	111.00

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	6417	0	6412	191	0
1	B	6423	0	6417	183	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	14	0	0
7	A	307	0	0	28	0
7	B	240	0	0	18	0
All	All	13497	0	12910	368	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 14.

All (368) 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: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: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:A:615:MET:CE	1:A:761:ILE:HG12	2.20	0.71
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.72	0.70
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:B:615:MET:CE	1:B:761:ILE:HG12	2.21	0.69
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:615:MET:HE1	1:A:761:ILE:HG12	1.73	0.68
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HG2	1:B:33:ARG:NH2	2.08	0.67
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: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: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: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: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: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:615:MET:HE3	1:A:615:MET:O	2.01	0.60
1:A:316:PHE:N	1:A:316:PHE:CD2	2.67	0.60
1:A:421:ASP:OD1	1:A:424:ARG:HD2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:615:MET:HE3	1:B:615:MET:O	2.02	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:204:GLY:C	1:B:205:LYS:HD2	2.24	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: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:421:ASP:CG	1:A:424:ARG:HB2	2.26	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:A:204:GLY:C	1:A:205:LYS:HD2	2.27	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:421:ASP:CG	1:B:424:ARG:HB2	2.27	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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:B:45:VAL:HG12	1:B:45:VAL:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:GLU:HG3	1:B:613:TYR:OH	2.11	0.50
1:A:795:LYS:HB2	7:A:2122:HOH:O	2.11	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:A:329:PHE:HB3	1:A:330:PRO:HD3	1.93	0.49
1:B:826:ASN:HD22	1:B:826:ASN:C	2.14	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:A:615:MET:HE2	1:A:761:ILE:HG12	1.93	0.48
1:A:645:LEU:HD11	1:A:652:LEU:HD11	1.90	0.48
1:B:157:TYR:HD2	1:B:303:THR:HG1	1.58	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:197:MET:HE2	1:A:224:LEU:HD13	1.95	0.48
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.49	0.48
1:A:494:LEU:HD23	1:A:494:LEU:C	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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
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: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: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:B:693:ASP:O	1:B:694:GLY:C	2.54	0.46
1:A:136:LEU:HD23	1:A:136:LEU:C	2.36	0.46
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.98	0.45
1:A:826:ASN:HD22	1:A:826:ASN:C	2.19	0.45
1:B:432:GLU:O	1:B:437:LYS:HA	2.17	0.45
1:B:738:LEU:HB2	1:B:777:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:GLN:HE21	1:B:76:ASP:CG	2.19	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:A:693:ASP:O	1:A:694:GLY:C	2.54	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: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:A:732:TYR:CD1	1:A:739:LYS:HA	2.52	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
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.82	0.44
1:A:592:LYS:HE2	1:A:592:LYS:C	2.38	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:592:LYS:HE2	1:B:592:LYS:C	2.38	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:732:TYR:CD1	1:B:739:LYS:HA	2.52	0.44
1:B:615:MET:HE2	1:B:761:ILE:HG12	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:555:VAL:HG12	1:A:556:LYS:N	2.33	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:B:615:MET:CE	1:B:618:MET:HB2	2.48	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: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: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
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:197:MET:HE2	1:B:224:LEU:HD13	2.01	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:382:GLU:CD	1:A:382:GLU:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ASN:HB3	1:B:561:SER:HB3	2.01	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:382:GLU:CD	1:B:382:GLU:H	2.22	0.42
1:B:713:MET:HB3	1:B:717:ASP:HB2	2.02	0.42
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	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:A:98:THR:O	1:A:102:LEU:HB2	2.18	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:136:LEU:C	1:B:136:LEU:HD23	2.40	0.41
1:B:283:ASP:O	1:B:284:ASN:HB2	2.20	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
1:A:315:LYS:O	1:A:316:PHE:C	2.58	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:494:LEU:C	1:B:494:LEU:HD23	2.40	0.41
1:B:525:LEU:HD23	1:B:802:LEU:HD23	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:ASP:C	1:B:769:ASP:OD1	2.58	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:197:MET:HE2	1:B:197:MET:HB2	1.83	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

### 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	784/847 (93%)	742 (95%)	39 (5%)	3 (0%)	30	29
1	B	785/847 (93%)	742 (94%)	39 (5%)	4 (0%)	25	23
All	All	1569/1694 (93%)	1484 (95%)	78 (5%)	7 (0%)	30	29

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 ⓘ

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	692/740 (94%)	662 (96%)	30 (4%)	25	25
1	B	693/740 (94%)	661 (95%)	32 (5%)	23	23
All	All	1385/1480 (94%)	1323 (96%)	62 (4%)	23	24

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	78	CYS
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	106	ASN
1	A	243	LEU
1	A	277	ARG
1	A	316	PHE
1	A	337	LEU
1	A	361	TRP
1	A	492	LEU
1	A	499	LEU
1	A	502	LEU
1	A	505	GLU
1	A	528	ASP
1	A	551	THR
1	A	573	TYR
1	A	576	GLN
1	A	577	LEU
1	A	592	LYS
1	A	613	TYR
1	A	622	LEU
1	A	628	ASP
1	A	645	LEU
1	A	683	LEU
1	A	733	GLU

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Mol	Chain	Res	Type
1	A	735	LEU
1	A	815	ARG
1	A	826	ASN
1	B	44	ASN
1	B	78	CYS
1	B	90	TYR
1	B	95	LEU
1	B	102	LEU
1	B	106	ASN
1	B	243	LEU
1	B	277	ARG
1	B	281	PRO
1	B	325	VAL
1	B	337	LEU
1	B	361	TRP
1	B	489	ARG
1	B	492	LEU
1	B	499	LEU
1	B	502	LEU
1	B	505	GLU
1	B	528	ASP
1	B	551	THR
1	B	573	TYR
1	B	576	GLN
1	B	577	LEU
1	B	592	LYS
1	B	613	TYR
1	B	622	LEU
1	B	628	ASP
1	B	645	LEU
1	B	683	LEU
1	B	733	GLU
1	B	735	LEU
1	B	815	ARG
1	B	826	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	72	GLN
1	A	97	ASN

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Mol	Chain	Res	Type
1	A	106	ASN
1	A	250	ASN
1	A	369	GLN
1	A	459	HIS
1	A	576	GLN
1	B	96	GLN
1	B	105	GLN
1	B	106	ASN
1	B	250	ASN
1	B	369	GLN
1	B	459	HIS
1	B	576	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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
5	RBF	A	859	-	29,29,29	1.61	9 (31%)	42,43,43	2.11	14 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	700	A	862	-	29,33,33	1.89	9 (31%)	39,47,47	1.57	6 (15%)
3	PLP	A	860	1	15,15,16	2.19	6 (40%)	21,22,23	1.35	3 (14%)
6	MRD	B	902	-	7,7,7	0.71	0	9,10,10	0.77	0
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
5	RBF	A	859	-	-	2/14/14/14	0/3/3/3
4	700	A	862	-	-	0/19/32/32	0/4/4/4
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
6	MRD	B	902	-	-	2/5/5/5	-
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 (30) 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	C5-C4	4.19	1.44	1.36
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
4	A	862	700	C7-C6	2.95	1.52	1.41
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	C2-C3	2.85	1.42	1.36
4	A	862	700	C13-C12	2.82	1.43	1.38
5	A	859	RBF	C9-C9A	2.71	1.44	1.39
2	A	861	NBG	C2-C1	2.67	1.55	1.53
5	A	859	RBF	C5'-C4'	2.60	1.58	1.52
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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 (24) 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
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
4	A	862	700	C7-C6-C1	-4.40	102.44	106.27
5	A	859	RBF	O4-C4-C4A	-4.20	115.44	126.53
2	A	861	NBG	C5-O5-C1	3.92	117.92	112.47
4	A	862	700	C8-C9-N1	3.73	122.36	115.19
4	A	862	700	C8-N2-C1	3.67	112.10	104.45
5	A	859	RBF	C5A-C9A-N10	-3.65	114.67	117.97
3	A	860	PLP	O3P-P-O4P	-2.89	99.13	106.67
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
3	A	860	PLP	C2A-C2-C3	2.32	123.51	120.80
4	A	862	700	C3-C2-C1	-2.30	118.05	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
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:

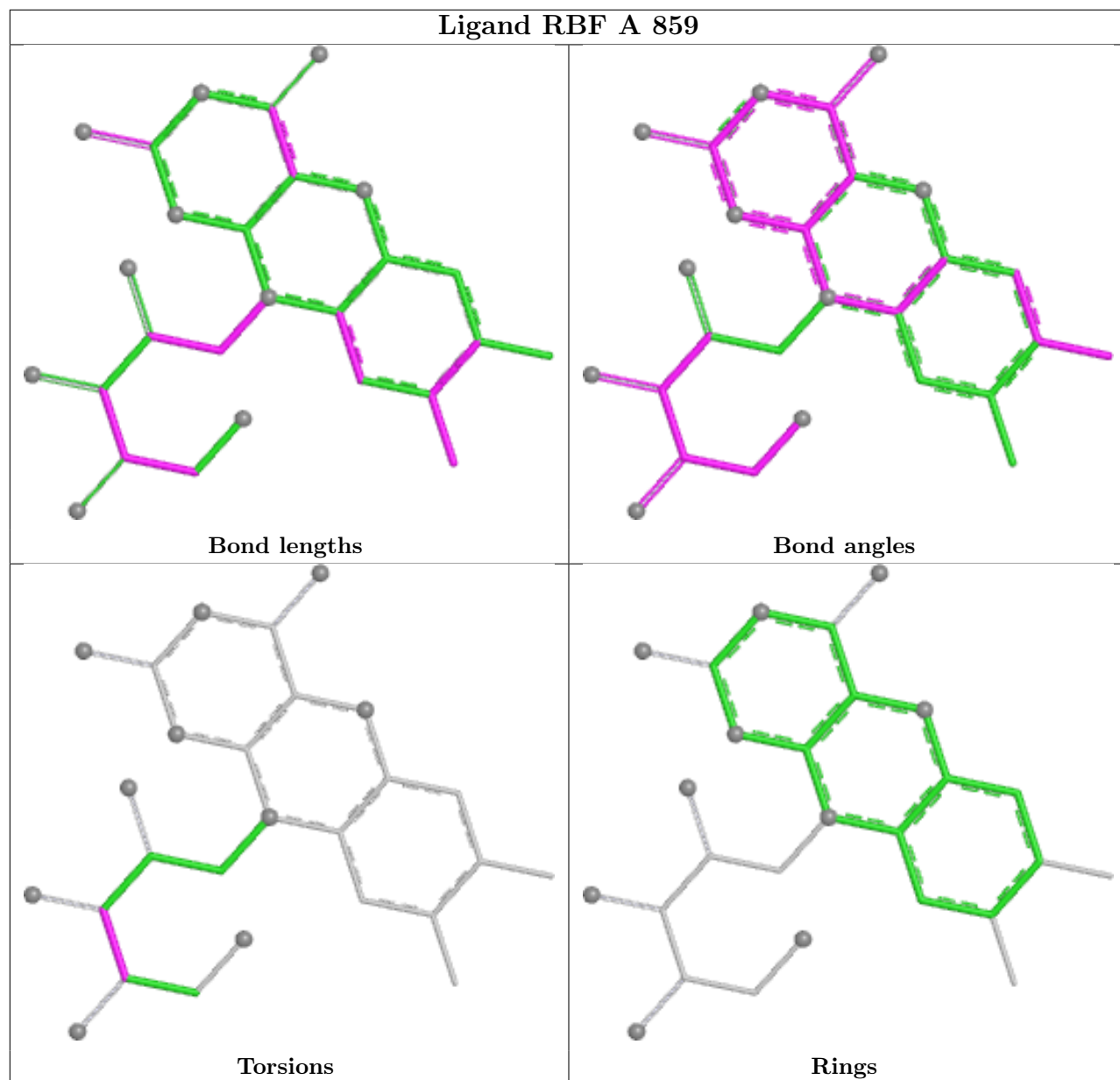
Mol	Chain	Res	Type	Atoms
3	B	860	PLP	C6-C5-C5A-O4P
3	B	860	PLP	C4-C5-C5A-O4P
6	B	902	MRD	C2-C3-C4-O4
6	B	902	MRD	C2-C3-C4-C5
5	A	859	RBF	O3'-C3'-C4'-C5'
5	A	859	RBF	O3'-C3'-C4'-O4'

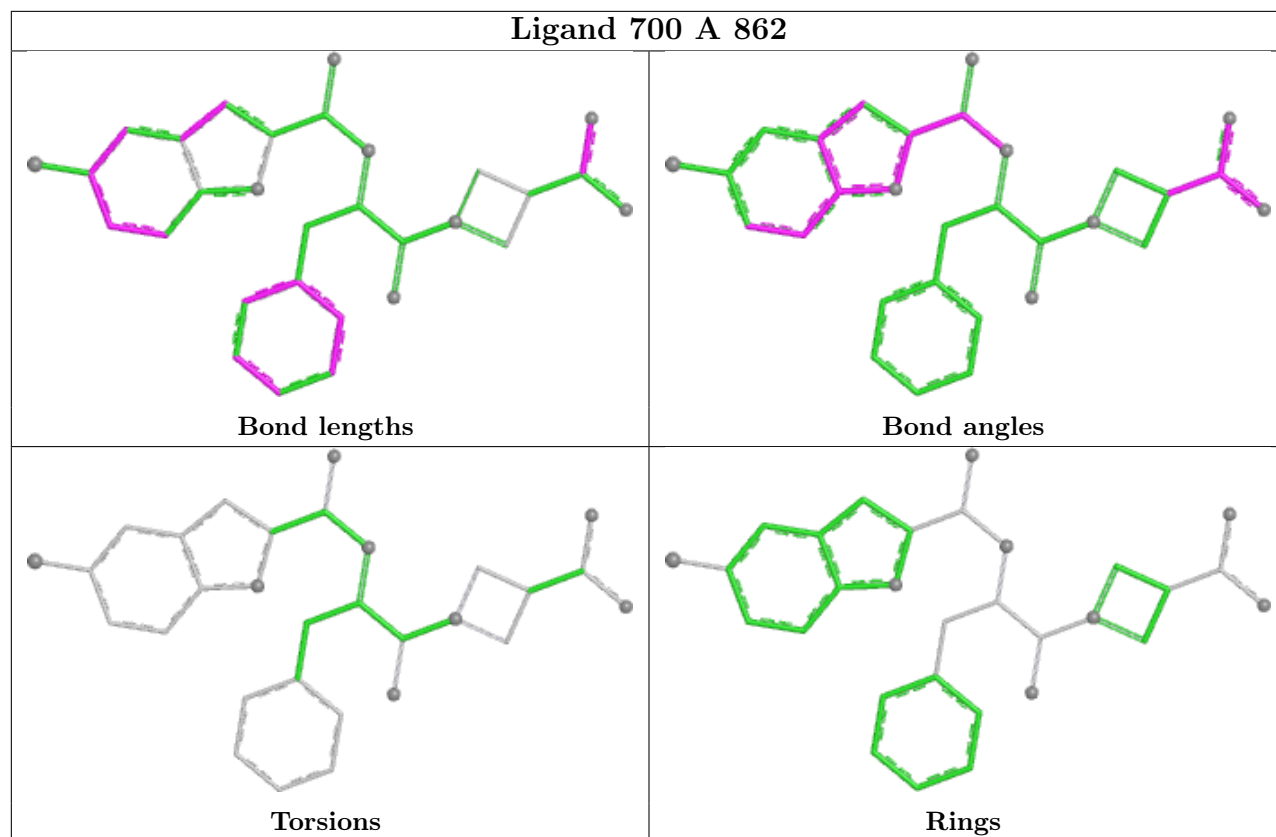
There are no ring outliers.

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.

## Ligand RBF A 859





## 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.