



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:39 AM GMT

PDB ID : 1L5R  
Title : Human liver glycogen phosphorylase a complexed with riboflavin, N-Acetyl-b  
eta-D-Glucopyranosylamineand 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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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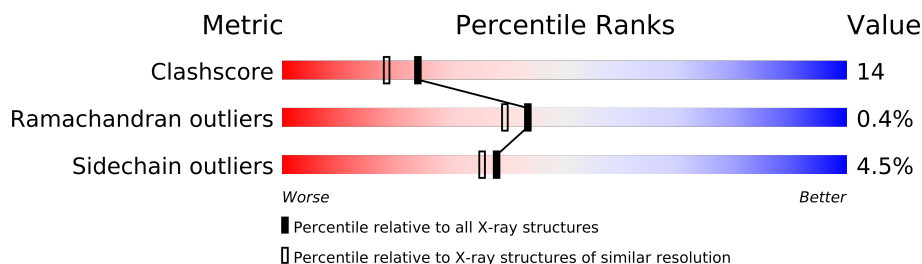
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

## 2 Entry composition i

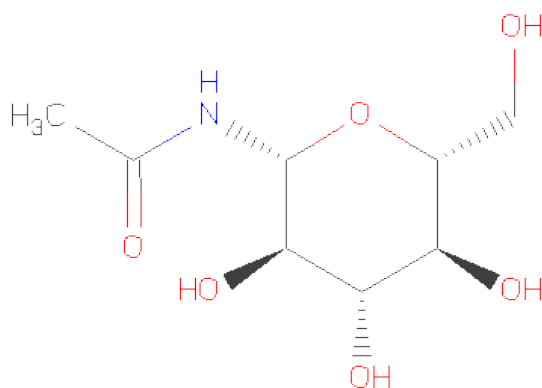
There are 7 unique types of molecules in this entry. The entry contains 13497 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula:  $C_8H_{15}NO_6$ ).



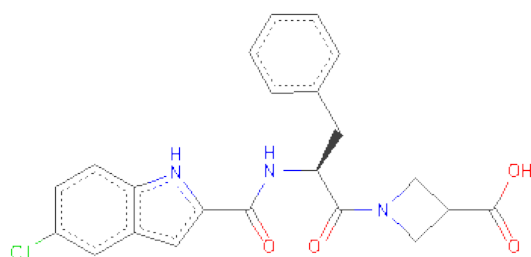
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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



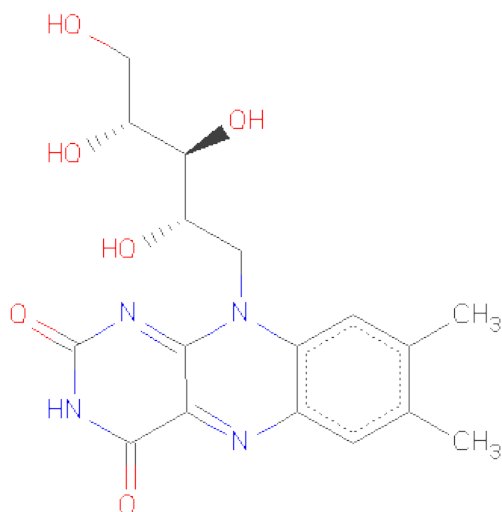
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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



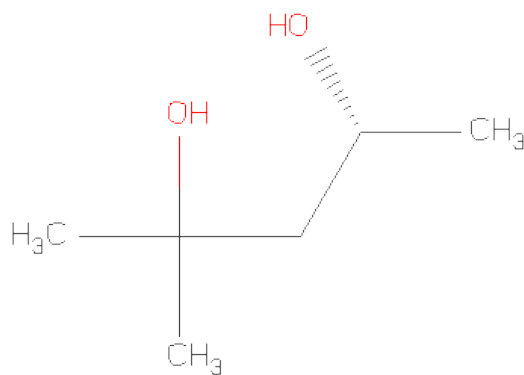
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			30	22	1	3	4		

- Molecule 5 is RIBOFLAVIN (three-letter code: RBF) (formula:  $C_{17}H_{20}N_4O_6$ ).



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

- 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
			Total	C	O		
6	B	1	8	6	2	0	0

- 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

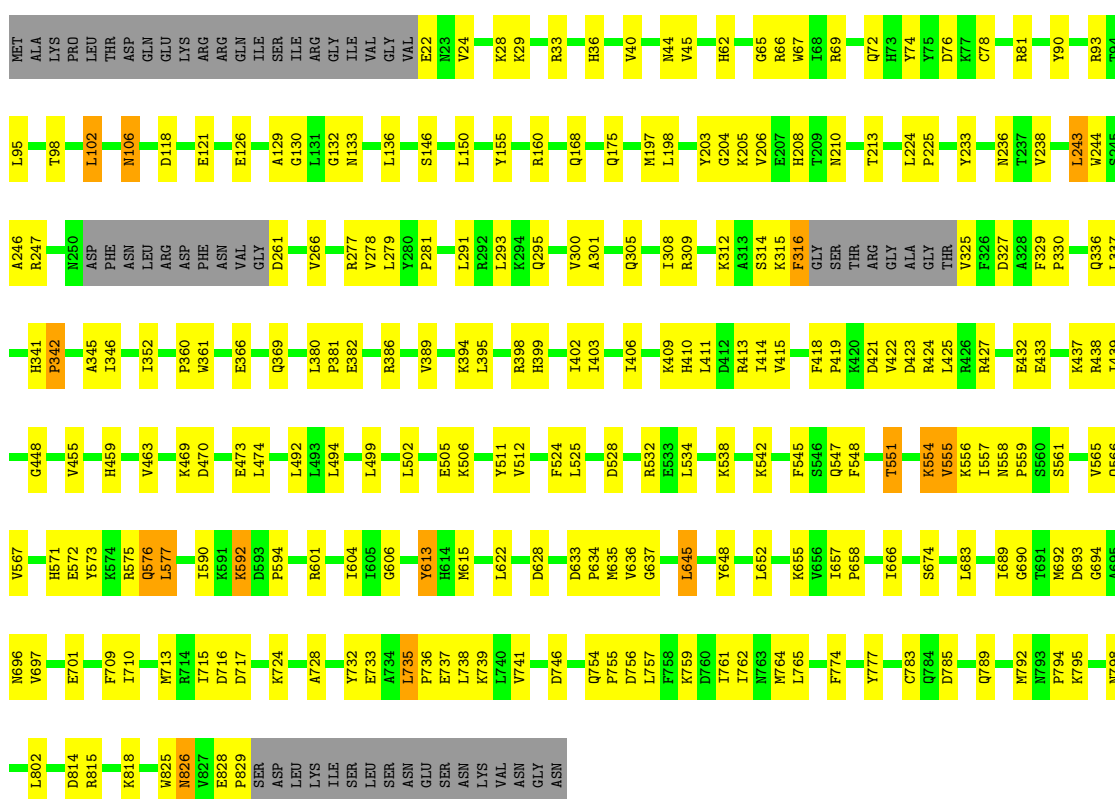
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

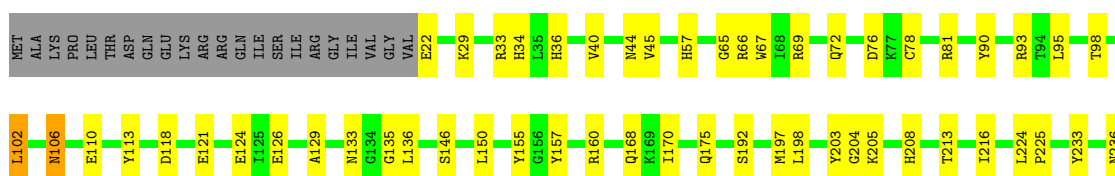
- Molecule 1: glycogen phosphorylase, liver form

Chain A:



- Molecule 1: glycogen phosphorylase, liver form

Chain B:



T237	V238	F329	P330	C445	V565	H691	D785
L243	V244	Q336	L337	G448	Q566	H692	K786
S245	A246	H341	P342	V455	V567	D693	Q789
R247		A345	I346	H459	H571	A695	M792
N250	ASP	I352	W361	V463	E572	N696	N793
PHE	ASN	E382	Y374	K469	Y573	V697	P794
LEU	ARG	R386	E382	D470	K574	E701	L802
ASP	ASN	V359	K394	E473	Q576	L708	D814
ARG	PHE	H399	H399	L474	L577	F709	R815
ASN	ASN	I402	I403	T487	K592	I710	K818
VAL	GLY	I406	I406	P488	D593	R713	W825
D261		K409	K409	R489	P594	I715	N826
V266		H410	H410	L492	V599	D716	N827
E273		L411	L411	L493	P600	D717	E828
R277		D412	D412	L494	I604	K724	P829
V278		R413	R413	L499	G606	A728	S830
P281		I414	I414	L502	Y613	Y732	ASP
N282		V415	V415	E505	H614	E733	LEU
D283		F418	F418	K506	M615	A734	LYS
N284		R420	R420	L502	M618	L735	ILE
F285		L425	L425	D528	L622	P736	SER
V300		R426	R426	R532	D628	E737	SER
A301		E427	E427	K538	D633	L738	ASN
A302		E432	E432	L542	P634	K739	GLU
I308		E433	E433	L543	V635	L740	ASN
R309		K437	K437	F544	G637	V741	LYS
F311		I439	I439	F545	L645	D746	VAL
K312				S546	E646	P752	ASN
A313				Q547	N647	K753	GLY
S314				F548	Y648	Q754	ASN
K315				T551	L652	P755	ASN
F316				K554	K655	L757	GLY
GLY				V555	V656	N758	ASN
SER				K556	I657	K759	ASN
THR				I557	P658	D760	ASN
ARG				N558	I666	I761	ASN
GLY				S561	S674	I762	ASN
ALA					L683	N763	ASN
GLY					I689	N764	ASN
THR					G690	L765	ASN
V325						D769	ASN
						F774	ASN
						Y777	ASN
						C783	ASN
						Q784	ASN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, RBF, 700, NBG, PLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.44	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
7	B	240	0	0	18	0
All	All	13497	0	12910	368	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (368) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:HH11	1:A:532:ARG:HB2	1.60	0.67
1:B:532:ARG:HB2	1:B:532:ARG:HH11	1.58	0.67
1:B:455:VAL:H	1:B:459:HIS:HD2	1.43	0.66
1:B:146:SER:O	1:B:150:LEU:HD13	1.95	0.66
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.29	0.66
1:A:594:PRO:HG3	1:A:635:MET:SD	2.34	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:594:PRO:HG3	1:B:635:MET:SD	2.37	0.65
1:B:415:VAL:HG22	1:B:425:LEU:HD11	1.79	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:455:VAL:H	1:A:459:HIS:HD2	1.43	0.64
1:A:409:LYS:O	1:A:413:ARG:HG2	1.97	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:CD2	1:A:316:PHE:N	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
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:204:GLY:C	1:B:205:LYS:HD2	2.24	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: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:735:LEU:HD23	1:A:777:TYR:HD2	1.70	0.56
1:A:330:PRO:HB2	7:A:2416:HOH:O	2.05	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
1:B:532:ARG:NH1	1:B:532:ARG:HB2	2.22	0.53
1:B:118:ASP:HA	7:B:2363:HOH:O	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:572:GLU:HG3	1:A:613:TYR:OH	2.08	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:HD22	1:A:106:ASN:N	2.06	0.53
1:A:532:ARG:NH1	1:A:532:ARG:HB2	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:HD2	1:A:316:PHE:N	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:B:308:ILE:HD12	1:B:352:ILE:HD13	1.92	0.52
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.40	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:B:459:HIS:O	1:B:463:VAL:HG23	2.10	0.51
1:A:233:TYR:CE2	1:A:512:VAL:HG11	2.46	0.51
1:B:410:HIS:O	1:B:414:ILE:HD13	2.09	0.51
1:A:208:HIS:ND1	1:A:213:THR:HG22	2.26	0.51
1:A:735:LEU:CD1	1:A:735:LEU:N	2.73	0.51
1:A:22:GLU:HB3	1:A:62:HIS:HE1	1.76	0.51
1:B:208:HIS:ND1	1:B:213:THR:HG22	2.25	0.51
1:B:735:LEU:CD1	1:B:735:LEU:N	2.74	0.51
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.93	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:168:GLN:HG3	1:B:175:GLN:HG3	1.92	0.50
1:B:67:TRP:HA	1:B:238:VAL:HB	1.93	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:764:MET:SD	1:B:765:LEU:HD12	2.52	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:300:VAL:HG13	1:B:345:ALA:HA	1.94	0.49
1:A:66:ARG:HD2	1:A:236:ASN: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:B:826:ASN:ND2	1:B:826:ASN:O	2.38	0.49
1:A:828:GLU:HG3	1:A:829:PRO:HD2	1.94	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: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:A:67:TRP:HA	1:A:238:VAL:HB	1.95	0.48
1:B:724:LYS:O	1:B:724:LYS:HD3	2.13	0.48
1:B:652:LEU:HD13	1:B:652:LEU:O	2.14	0.48
1:B:198:LEU:HD21	1:B:309:ARG:CZ	2.44	0.48
1:A:494:LEU:HD23	1:A:494:LEU:C	2.34	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:556:LYS:HD3	1:A:557:ILE:N	2.28	0.48
1:A:133:ASN:OD1	1:A:281:PRO:HA	2.14	0.48
1:A:65:GLY:O	1:A:69:ARG:HG3	2.14	0.48
1:A:689:ILE:O	1:A:689:ILE:HG23	2.14	0.48
1:A:45:VAL:O	1:A:45:VAL:HG12	2.14	0.48
1:B:205:LYS:HG3	7:B:2302:HOH:O	2.13	0.47
1:B:689:ILE:HG23	1:B:689:ILE:O	2.14	0.47
1:A:386:ARG:HA	1:A:439:ILE:O	2.14	0.47
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.44	0.47
1:A:724:LYS:O	1:A:724:LYS:HD3	2.14	0.47
1:A:301:ALA:O	1:A:305:GLN:HG3	2.13	0.47
1:B:645:LEU:HD11	1:B:652:LEU:HD11	1.94	0.47
1:B:65:GLY:O	1:B:69:ARG:HG3	2.15	0.47
1:A:577:LEU:CD1	1:A:765:LEU:HD11	2.44	0.47
1:A:545:PHE:O	1:A:548:PHE:HB3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:ILE:CG2	1:A:425:LEU:HD23	2.45	0.47
1:A:261:ASP:N	7:A:2495:HOH:O	2.47	0.47
1:B:532:ARG:CB	1:B:532:ARG:NH1	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:746:ASP:HB2	1:A:762:ILE:HG13	1.97	0.47
1:A:511:TYR:N	7:A:2148:HOH:O	2.47	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:571:HIS:H	1:A:576:GLN:NE2	2.12	0.46
1:A:293:LEU:HG	1:A:395:LEU:HD23	1.96	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: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:402:ILE:O	1:A:406:ILE:HG13	2.15	0.46
1:A:592:LYS:HE2	1:A:592:LYS:O	2.15	0.46
1:A:398:ARG:O	1:A:402:ILE:HG13	2.16	0.46
1:B:225:PRO:HB3	1:B:244:TRP:CZ3	2.51	0.46
1:A:633:ASP:O	1:A:636:VAL:HG22	2.15	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:566:GLN:HA	7:B:2012:HOH:O	2.15	0.46
1:B:402:ILE:O	1:B:406:ILE:HG13	2.16	0.46
1:B:693:ASP:O	1:B:694:GLY:C	2.54	0.46
1:B:576:GLN:H	1:B:576:GLN:NE2	2.13	0.46
1:A:575:ARG:HD3	1:A:666:ILE:O	2.15	0.46
1:A:136:LEU:C	1:A:136:LEU:HD23	2.36	0.46
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
1:A:826:ASN:C	1:A:826:ASN:HD22	2.19	0.45
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.98	0.45
1:B:648:TYR:HD1	1:B:652:LEU:HD12	1.81	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:728:ALA:HB1	1:B:774:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:633:ASP:O	1:B:636:VAL:HG22	2.16	0.45
1:B:433:GLU:HG3	1:B:437:LYS:HG2	1.99	0.45
1:B:414:ILE:CG2	1:B:425:LEU:HD23	2.45	0.45
1:B:715:ILE:HG23	1:B:716:ASP:N	2.31	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:592:LYS:O	1:B:592:LYS:HE2	2.15	0.45
1:A:693:ASP:O	1:A:694:GLY:C	2.54	0.45
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.98	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: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:168:GLN:HG3	1:A:175:GLN:HG3	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:525:LEU:HD23	1:A:802:LEU:HD23	1.99	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:HB3	1:B:438:ARG:HE	1.60	0.45
1:B:81:ARG:HD3	1:B:155:TYR:CE2	2.52	0.44
1:A:592:LYS:C	1:A:592:LYS:HE2	2.38	0.44
1:B:592:LYS:C	1:B:592:LYS:HE2	2.38	0.44
1:B:315:LYS:HG3	1:B:315:LYS:O	2.17	0.44
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.82	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:B:308:ILE:O	1:B:312:LYS:HG3	2.17	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: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:B:424:ARG:HH22	1:B:474:LEU:CD1	2.30	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:A:336:GLN:OE1	1:A:825:TRP:NE1	2.45	0.43
1:A:308:ILE:HD12	1:A:352:ILE:HD13	2.00	0.43
1:A:81:ARG:HD3	1:A:155:TYR:CE2	2.53	0.43
1:A:555:VAL:HG12	1:A:556:LYS:N	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.99	0.43
1:B:575:ARG:HD3	1:B:666:ILE:O	2.18	0.43
1:B:567:VAL:HA	1:B:606:GLY:O	2.18	0.43
1:B:386:ARG:HA	1:B:439:ILE:O	2.17	0.43
1:B:36:HIS:O	1:B:40:VAL:HA	2.19	0.43
1:B:615:MET:CE	1:B:618:MET:HB2	2.48	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: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:A:566:GLN:HA	7:A:2057:HOH:O	2.18	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:B:828:GLU:CG	1:B:829:PRO:HD2	2.47	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:792:MET:O	1:B:794:PRO:HD3	2.18	0.43
1:B:336:GLN:OE1	1:B:825:TRP:NE1	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:B:197:MET:HE2	1:B:224:LEU:HD13	2.01	0.42
1:B:754:GLN:N	1:B:755:PRO:HD3	2.34	0.42
1:A:24:VAL:O	1:A:28:LYS:HG3	2.18	0.42
1:A:360:PRO:HB2	7:A:2441:HOH:O	2.19	0.42
1:A:382:GLU:H	1:A:382:GLU:CD	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
1:B:558:ASN:HB3	1:B:561:SER:HB3	2.01	0.42
1:A:735:LEU:HD23	1:A:777:TYR:CD2	2.52	0.42
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.01	0.42
1:A:735:LEU:N	1:A:735:LEU:HD12	2.35	0.42
1:A:554:LYS:O	1:A:555:VAL:O	2.38	0.42
1:A:36:HIS:O	1:A:40:VAL:HA	2.19	0.42
1:B:713:MET:HB3	1:B:717:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:382:GLU:CD	1:B:382:GLU:H	2.22	0.42
1:A:210:ASN:ND2	7:A:2270:HOH:O	2.53	0.42
1:B:233:TYR:CD2	1:B:513:LYS:HE3	2.55	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.20	0.42
1:A:557:ILE:O	1:A:559:PRO:HD3	2.20	0.42
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.23	0.42
1:B:657:ILE:HB	1:B:658:PRO:HD3	2.02	0.41
1:A:98:THR:O	1:A:102:LEU:HB2	2.18	0.41
1:B:761:ILE:O	1:B:765:LEU:HD13	2.19	0.41
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.86	0.41
1:A:300:VAL:HG13	1:A:345:ALA:HA	2.02	0.41
1:A:433:GLU:HG3	1:A:437:LYS:HG2	2.01	0.41
1:B:283:ASP:O	1:B:284:ASN:HB2	2.20	0.41
1:B:136:LEU:HD23	1:B:136:LEU:C	2.40	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:OE1	1:B:22:GLU:HA	2.20	0.41
1:A:315:LYS:O	1:A:316:PHE:C	2.58	0.41
1:B:735:LEU:HD23	1:B:777:TYR:CD2	2.54	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.36	0.41
1:A:315:LYS:HG3	1:A:315:LYS:O	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:B:494:LEU:HD23	1:B:494:LEU:C	2.40	0.41
1:B:636:VAL:CG2	1:B:637:GLY:N	2.84	0.41
1:B:233:TYR:CZ	1:B:512:VAL:HG11	2.56	0.41
1:B:246:ALA:O	1:B:273:GLU:HG2	2.21	0.41
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.51	0.41
1:A:281:PRO:HD2	7:A:2410:HOH:O	2.20	0.40
1:B:561:SER:HA	1:B:600:PRO:HG2	2.03	0.40
1:A:291:LEU:O	1:A:295:GLN:HG3	2.21	0.40
1:B:769:ASP:C	1:B:769:ASP:OD1	2.58	0.40
1:B:203:TYR:HE2	1:B:394:LYS:HD2	1.86	0.40
1:A:601:ARG:HG3	7:A:2212:HOH:O	2.21	0.40
1:A:655:LYS:O	1:A:658:PRO:HD2	2.21	0.40
1:B:555:VAL:CG1	1:B:556:LYS:N	2.84	0.40
1:B:282:ASN:HB3	1:B:285:PHE:HB3	2.04	0.40
1:A:418:PHE:N	1:A:419:PRO:HD3	2.36	0.40
1:B:692:MET:HG3	1:B:697:VAL:HG22	2.03	0.40
1:B:34:HIS:CE1	1:B:57:HIS:HB3	2.56	0.40
1:B:197:MET:HB2	1:B:197:MET:HE2	1.83	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	43	39
1	B	785/847 (93%)	742 (94%)	39 (5%)	4 (0%)	38	33
All	All	1569/1694 (93%)	1484 (95%)	78 (5%)	7 (0%)	43	39

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%)	40	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	693/740 (94%)	661 (95%)	32 (5%)	37	34
All	All	1385/1480 (94%)	1323 (96%)	62 (4%)	38	35

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
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

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Mol	Chain	Res	Type
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

Some 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
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

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Mol	Chain	Res	Type
1	B	369	GLN
1	B	459	HIS
1	B	576	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	2.34	9 (31%)	39,43,43	3.11	12 (30%)
3	PLP	A	860	1	14,15,16	1.67	3 (21%)	20,22,23	1.32	4 (20%)
2	NBG	A	861	-	15,15,15	1.32	2 (13%)	21,21,21	1.22	2 (9%)
4	700	A	862	-	33,33,33	1.84	11 (33%)	47,47,47	1.12	4 (8%)
3	PLP	B	860	1	14,15,16	1.64	2 (14%)	20,22,23	0.91	0
6	MRD	B	902	-	7,7,7	0.64	0	10,10,10	0.78	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	-	-	0/14/14/14	0/0/3/3
3	PLP	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	700	A	862	-	-	1/22/32/32	0/1/4/4
3	PLP	B	860	1	-	0/6/6/8	0/1/1/1
6	MRD	B	902	-	-	0/5/5/5	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	859	RBF	C4-C4A	6.76	1.52	1.41
3	B	860	PLP	C3-C2	-4.91	1.37	1.40
5	A	859	RBF	C1'-C2'	4.86	1.56	1.51
5	A	859	RBF	C1'-N10	4.60	1.53	1.48
4	A	862	700	C8-N2	-4.12	1.32	1.36
5	A	859	RBF	C5A-N5	3.70	1.41	1.35
4	A	862	700	C22-C20	3.42	1.59	1.54
4	A	862	700	C5-C4	3.36	1.44	1.36
3	A	860	PLP	C5A-C5	3.24	1.59	1.51
4	A	862	700	C3-C4	3.05	1.44	1.38
4	A	862	700	C2-C3	2.95	1.42	1.36
4	A	862	700	C7-C6	2.94	1.52	1.41
5	A	859	RBF	C4A-N5	-2.94	1.30	1.36
2	A	861	NBG	C2-C1	2.89	1.55	1.52
5	A	859	RBF	C8M-C8	2.73	1.56	1.51
4	A	862	700	C16-C11	2.51	1.44	1.38
5	A	859	RBF	C8-C7	2.42	1.47	1.40
2	A	861	NBG	C1-N1	2.39	1.46	1.43
5	A	859	RBF	C9A-N10	2.32	1.42	1.38
3	A	860	PLP	C2-N1	2.23	1.38	1.33
4	A	862	700	C12-C11	2.20	1.43	1.38
3	A	860	PLP	P-O3P	-2.20	1.46	1.54
5	A	859	RBF	C5'-C4'	2.18	1.58	1.52
4	A	862	700	O4-C21	-2.12	1.22	1.30
4	A	862	700	C15-C14	2.09	1.43	1.37
3	B	860	PLP	P-O3P	-2.08	1.47	1.54
4	A	862	700	C13-C12	2.04	1.43	1.39

All (22) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	859	RBF	C2-N1-C10	11.72	126.79	114.98
5	A	859	RBF	C4A-C10-N10	-9.01	116.02	120.51
5	A	859	RBF	O5'-C5'-C4'	-5.60	98.52	111.05
5	A	859	RBF	O4'-C4'-C3'	4.86	121.16	109.05
5	A	859	RBF	C10-C4A-N5	4.33	125.71	120.45
2	A	861	NBG	C5-O5-C1	3.90	117.92	112.50
5	A	859	RBF	C4A-C10-N1	-3.61	119.13	122.73
5	A	859	RBF	N1-C10-N10	3.38	124.86	115.97
4	A	862	700	O3-C21-C20	-2.92	115.29	122.80
3	A	860	PLP	O3P-P-O2P	2.77	118.38	107.61
4	A	862	700	O4-C21-O3	2.75	130.29	124.07
3	A	860	PLP	O3P-P-O4P	-2.73	99.13	106.65
4	A	862	700	C8-C9-N1	2.54	122.36	116.55
5	A	859	RBF	O4'-C4'-C5'	-2.53	103.29	109.20
4	A	862	700	C4-C5-C6	-2.46	117.49	119.22
5	A	859	RBF	N3-C2-N1	-2.25	116.41	121.19
3	A	860	PLP	O3-C3-C2	2.22	121.56	117.61
5	A	859	RBF	C5A-C9A-N10	-2.17	114.67	116.80
5	A	859	RBF	C1'-N10-C10	-2.15	116.11	119.17
3	A	860	PLP	C2A-C2-C3	2.05	123.51	121.02
5	A	859	RBF	C9-C9A-C5A	2.04	122.79	119.38
2	A	861	NBG	C2-C1-N1	-2.01	108.72	111.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	862	700	C17-C18-N3-C22

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.