



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:13 PM GMT

PDB ID : 1EM6  
Title : HUMAN LIVER GLYCOGEN PHOSPHORYLASE A COMPLEXED WITH GLCNAC AND CP-526,423  
Authors : Rath, V.L.; Ammirati, M.; Danley, D.E.; Ekstrom, J.L.; Hynes, T.R.; Olson, T.V.; Hoover, D.J.  
Deposited on : 2000-03-16  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

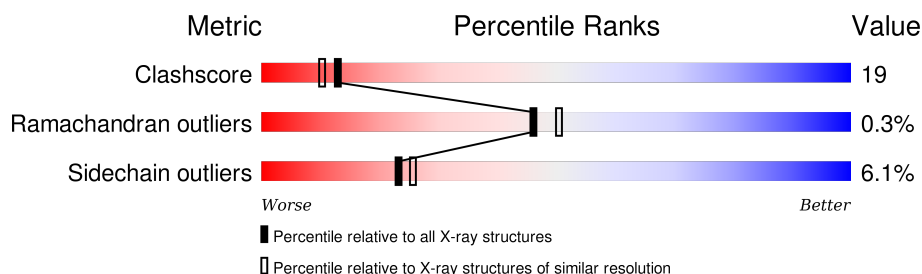
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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	B	1902	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13599 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.

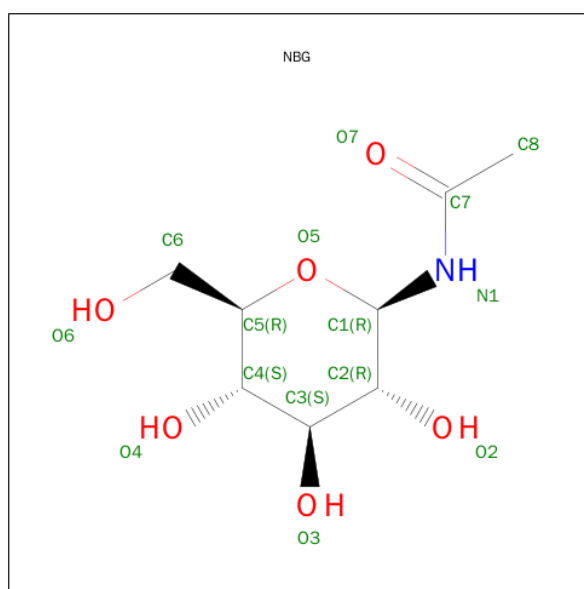
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	29			
1	B	787	Total	C	N	O	S	0	0	0
			6380	4097	1082	1172	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 SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



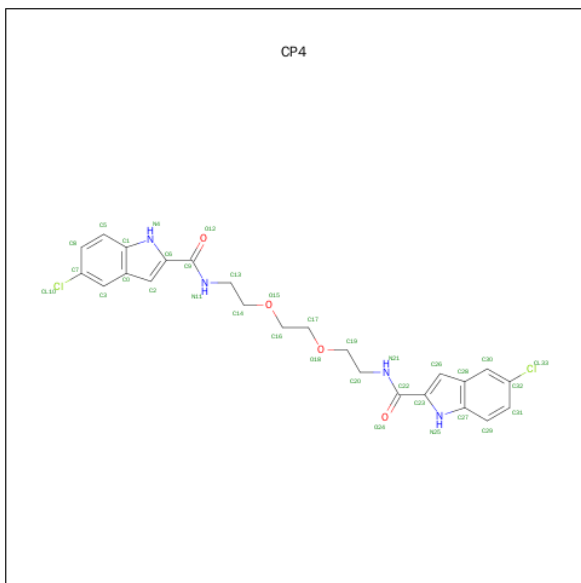
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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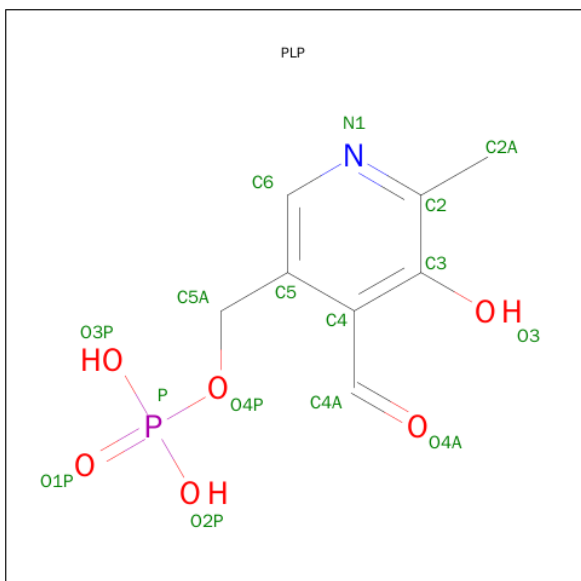
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is BIS[5-CHLORO-1H-INDOL-2-YL-CARBONYL-AMINOETHYL]-ETHYLEN E GLYCOL (three-letter code: CP4) (formula: C<sub>24</sub>H<sub>24</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			34	24	2	4	4	

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	379	Total	O	0	0
			379	379		
6	B	358	Total	O	0	0
			358	358		



LEU	L735	L652	V565	E473	E382	R292	D181	R81
SER	F736	V656	Q566	E483	E385	Q295	D184	V62
ASN	I745	I657	K568	R483	R386	E296	R184	Y83
GLU	D746	P658	R569	P488	V389	V300	R193	Y90
SER	F750	T660	H571	R489	L395	L304	F196	R92
ASN	Q754	D661	Y572	R490	L396	L308	N210	R93
ASN	F755	L662	K574	L492	P397	R309	T211	Y94
GLY	D756	G670	R575	L494	R398	R310	K214	Q96
ASN	L757	T671	Q576	L499	H399	F311	K215	I100
	F758	B672	L577	A500	I402	K312	I216	H101
	K759	A673	C580	E501	I403	A313	P225	L102
	I762	S674	L502	L502	E405	S314		N106
	K763	N678	P584	E505	I406	PHE	N235	D109
	M764	N679	LYS	K506	N407	GLY	N236	E110
	L765	K680	LYS	K507	Q408	SER	T237	A111
	F766	P681	LEU	I507	K409	THR	V238	I112
	Y767	N682	F598	E509	H410	ARG	L243	L115
	H768	L683		D510	I414	ALA	G115	G116
	F774	L687	R601	N511	V415	GLY	I244	L117
	Y777	T688	I605	N512	A416	T324	R247	I118
	I689	G690	G606	Q517	P419	V325	A248	I119
	K782	G690	K608	K520	K420	D327	P249	E126
	C783	D693	Y613	L521	V422	A328	ASN	E127
	Q784	N696	H614	F524	D423	F329	ASP	D128
	D785	V697	M615	D527	R424	P330	PHE	A129
	F786	B698		L531	L425	Q336	ASN	N133
	S788	E701	I619	K536	R426	D339	ARG	L136
	Q789	E702	K621	E539	M428	P342	ASP	F143
	L790	L708	I620	Q539	I431	A345	VAL	M147
	Y791	F709	I623	E540	E432	I346	D261	L152
	N792	I710	V626	N541	E433	P347	I263	A153
	F797	G712	A627	L542	G435	E348	N270	A154
	L802	M713	D628	L543	S436	D355	I274	Y155
	K810	D717	V630	F544	K437	R361	I275	R160
	R815	A720	N631	S546	I439	E366	S276	Y161
	T816	K723	D633	Q547	G448	L367	R277	E162
	I817	Y726	V636	F548	S449	K370	V278	Y163
	V827	E727	G637	T551	H450	A373	Y280	Q168
	E828	A728	V642	K554	V455		P281	K169
	P829	K729	I643	V555	I458		N284	I170
	S830	E730	F644	N558	H459		F285	R171
	ASP	Y731	E646	S561	K466		P286	W174
	LEU	Y732	N647	Y648			L291	E178
	LYS	E733	Y648	R649				
	I1E							
	SER	A734						

## 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, $\alpha$ , $\beta$ , $\gamma$	123.31Å 123.31Å 122.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.20	Depositor
% Data completeness (in resolution range)	92.7 (99.00-2.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.233 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: CP4, MPD, 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	0.35	0/6522	0.60	0/8822
1	B	0.35	0/6522	0.60	0/8822
All	All	0.35	0/13044	0.60	0/17644

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	6380	0	6361	236	2
1	B	6380	0	6361	258	1
2	A	15	0	15	1	0
2	B	15	0	15	1	0
3	A	34	0	24	0	0
4	A	15	0	7	0	0
4	B	15	0	6	0	0
5	B	8	0	14	0	0
6	A	379	0	0	21	0
6	B	358	0	0	32	1
All	All	13599	0	12803	490	2

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 19.

All (490) 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:133:ASN:HD22	1:B:569:ARG:NH2	1.56	1.02
1:B:789:GLN:HA	1:B:789:GLN:HE21	1.24	1.02
1:A:133:ASN:HD22	1:A:569:ARG:NH2	1.60	1.00
1:A:789:GLN:HA	1:A:789:GLN:HE21	1.24	0.98
1:A:133:ASN:HD21	1:A:281:PRO:HA	1.29	0.97
1:B:133:ASN:HD21	1:B:281:PRO:HA	1.30	0.93
1:B:662:LEU:HD12	1:B:787:VAL:HG11	1.52	0.89
1:B:379:VAL:HA	6:B:2254:HOH:O	1.74	0.86
1:A:662:LEU:HD12	1:A:787:VAL:HG11	1.56	0.85
1:A:163:TYR:CE1	1:A:181:ASP:HB3	2.12	0.85
1:B:678:ASN:HD22	1:B:679:MET:H	1.21	0.85
1:B:163:TYR:CE1	1:B:181:ASP:HB3	2.12	0.84
1:A:678:ASN:HD22	1:A:679:MET:H	1.25	0.84
1:B:133:ASN:HD22	1:B:569:ARG:HH22	1.22	0.83
1:A:29:LYS:HE2	1:A:33:ARG:NH1	1.94	0.83
1:A:133:ASN:HD22	1:A:569:ARG:HH22	1.25	0.82
1:B:29:LYS:HE2	1:B:33:ARG:NH1	1.96	0.81
1:B:168:GLN:HE21	1:B:647:ASN:H	1.28	0.81
1:B:378:THR:HG21	6:B:2357:HOH:O	1.80	0.80
1:B:324:THR:HG23	6:B:2486:HOH:O	1.81	0.80
1:B:378:THR:HA	6:B:2008:HOH:O	1.82	0.79
1:A:168:GLN:HE21	1:A:647:ASN:H	1.26	0.79
1:A:274:ASN:HD21	1:B:270:ASN:HD21	1.29	0.78
1:A:660:THR:HG21	1:A:681:PHE:HE2	1.49	0.78
1:B:210:ASN:N	1:B:210:ASN:HD22	1.82	0.78
1:B:547:GLN:O	1:B:551:THR:HG23	1.83	0.78
1:A:547:GLN:O	1:A:551:THR:HG23	1.83	0.77
1:B:662:LEU:HD21	1:B:689:ILE:CG2	2.15	0.76
1:A:797:TRP:HZ3	6:A:2328:HOH:O	1.68	0.76
1:A:555:VAL:HG21	1:A:643:ILE:HD11	1.68	0.75
1:A:109:ASP:HB3	6:A:2581:HOH:O	1.86	0.75
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.69	0.75
1:A:270:ASN:HD21	1:B:274:ASN:HD21	1.32	0.75
1:B:797:TRP:HZ3	6:B:2580:HOH:O	1.69	0.75
1:B:660:THR:HG21	1:B:681:PHE:HE2	1.52	0.74
1:A:662:LEU:HD21	1:A:689:ILE:CG2	2.17	0.74
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:HB3	1:A:494:LEU:HD21	1.69	0.73
1:A:210:ASN:N	1:A:210:ASN:HD22	1.84	0.72
1:B:96:GLN:HB3	1:B:494:LEU:HD21	1.69	0.72
1:B:555:VAL:HG21	1:B:643:ILE:HD11	1.70	0.72
1:B:678:ASN:HD22	1:B:679:MET:N	1.88	0.71
1:B:163:TYR:HE1	1:B:181:ASP:HB3	1.52	0.71
1:B:366:GLU:HG3	1:B:367:LEU:N	2.05	0.71
1:A:366:GLU:HG3	1:A:367:LEU:N	2.04	0.71
1:B:629:VAL:HG11	1:B:750:PHE:CD1	2.26	0.70
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.56	0.70
1:B:789:GLN:HA	1:B:789:GLN:NE2	2.04	0.70
1:A:629:VAL:HG11	1:A:750:PHE:CD1	2.26	0.70
1:A:163:TYR:HE1	1:A:181:ASP:HB3	1.54	0.69
1:A:756:ASP:HB3	6:A:2336:HOH:O	1.91	0.69
1:A:41:LYS:HD2	1:A:45:VAL:HG23	1.75	0.69
1:A:678:ASN:HD22	1:A:679:MET:N	1.90	0.69
1:A:789:GLN:HA	1:A:789:GLN:NE2	2.04	0.69
1:A:415:VAL:HG12	1:A:425:LEU:HD11	1.74	0.69
1:B:415:VAL:HG12	1:B:425:LEU:HD11	1.75	0.68
1:B:355:ASP:OD2	1:B:398:ARG:HD3	1.93	0.68
1:A:501:GLU:HG2	1:A:505:GLU:OE1	1.94	0.67
1:B:662:LEU:HD21	1:B:689:ILE:HG22	1.75	0.67
1:B:580:CYS:SG	1:B:622:LEU:HD13	2.35	0.67
1:A:262:TYR:CD2	1:A:263:ILE:HD12	2.30	0.67
1:B:501:GLU:HG3	6:B:2529:HOH:O	1.94	0.67
1:B:262:TYR:CD2	1:B:263:ILE:HD12	2.30	0.66
1:B:501:GLU:HG2	1:B:505:GLU:OE1	1.94	0.66
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.78	0.66
1:B:810:LYS:O	1:B:815:ARG:HD3	1.95	0.66
1:B:41:LYS:HD2	1:B:45:VAL:HG23	1.76	0.66
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.59	0.66
1:B:759:LYS:HE2	6:B:2111:HOH:O	1.96	0.65
1:A:810:LYS:O	1:A:815:ARG:HD3	1.96	0.65
1:B:509:GLU:O	1:B:512:VAL:HG22	1.96	0.65
1:A:174:TRP:CE2	1:A:621:LYS:HG3	2.31	0.65
1:A:355:ASP:OD2	1:A:398:ARG:HD3	1.95	0.65
1:B:174:TRP:CE2	1:B:621:LYS:HG3	2.31	0.65
1:B:678:ASN:ND2	1:B:679:MET:H	1.93	0.65
1:A:66:ARG:CD	1:A:236:ASN:HA	2.27	0.65
1:B:66:ARG:CD	1:B:236:ASN:HA	2.27	0.65
1:A:662:LEU:HD21	1:A:689:ILE:HG22	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.77	0.64
1:B:81:ARG:NH1	1:B:155:TYR:OH	2.31	0.64
1:B:61:ASP:O	1:B:64:VAL:HG22	1.98	0.63
1:B:630:VAL:HG21	1:B:642:VAL:HG23	1.81	0.63
1:A:450:HIS:HD2	6:A:2481:HOH:O	1.81	0.63
1:A:509:GLU:O	1:A:512:VAL:HG22	1.98	0.63
1:B:745:ILE:HG13	1:B:762:ILE:HD11	1.81	0.63
1:B:262:TYR:HD2	1:B:263:ILE:HD12	1.64	0.63
1:A:506:LYS:HD2	1:A:524:PHE:CE2	2.34	0.63
1:B:29:LYS:HE2	1:B:33:ARG:HH11	1.63	0.62
1:B:361:TRP:CZ3	1:B:409:LYS:HD3	2.34	0.62
1:A:170:ILE:O	1:A:171:ARG:HD2	1.99	0.62
1:B:455:VAL:H	1:B:459:HIS:HD2	1.46	0.62
1:A:262:TYR:HD2	1:A:263:ILE:HD12	1.65	0.62
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.35	0.62
1:A:29:LYS:HE2	1:A:33:ARG:HH11	1.63	0.61
1:A:745:ILE:HG13	1:A:762:ILE:HD11	1.81	0.61
1:B:571:HIS:H	1:B:576:GLN:NE2	1.98	0.61
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.81	0.61
1:A:361:TRP:CZ3	1:A:409:LYS:HD3	2.36	0.61
1:A:455:VAL:H	1:A:459:HIS:HD2	1.47	0.61
1:B:170:ILE:O	1:B:171:ARG:HD2	2.00	0.61
1:B:633:ASP:O	1:B:636:VAL:HG22	2.01	0.60
1:B:469:LYS:O	1:B:473:GLU:HG3	2.01	0.60
1:B:310:ARG:HD3	6:B:2366:HOH:O	2.02	0.60
1:B:450:HIS:HE1	6:B:2224:HOH:O	1.84	0.60
1:A:662:LEU:HD21	1:A:689:ILE:HG21	1.83	0.60
1:A:678:ASN:ND2	1:A:679:MET:H	1.97	0.60
1:B:450:HIS:HD2	6:B:2553:HOH:O	1.84	0.60
1:A:662:LEU:C	1:A:662:LEU:HD23	2.22	0.60
1:A:61:ASP:O	1:A:64:VAL:HG22	2.01	0.60
1:A:633:ASP:O	1:A:636:VAL:HG22	2.02	0.60
1:A:64:VAL:HG23	1:A:65:GLY:N	2.17	0.60
1:A:580:CYS:SG	1:A:622:LEU:HD13	2.42	0.60
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.83	0.60
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.85	0.60
1:B:662:LEU:C	1:B:662:LEU:HD23	2.21	0.60
1:A:571:HIS:H	1:A:576:GLN:NE2	1.99	0.60
1:A:274:ASN:ND2	1:A:277:ARG:HH21	2.00	0.60
1:A:152:LEU:HD22	1:A:827:VAL:CG1	2.32	0.59
1:A:205:LYS:HG3	6:A:2394:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD22	1:B:827:VAL:CG1	2.33	0.59
1:B:727:GLU:HG3	1:B:729:LYS:HG2	1.84	0.59
1:A:124:GLU:HG2	6:A:2701:HOH:O	2.02	0.59
1:B:662:LEU:HD21	1:B:689:ILE:HG21	1.83	0.59
1:B:133:ASN:ND2	1:B:569:ARG:HH22	1.95	0.59
1:A:81:ARG:NH1	1:A:155:TYR:OH	2.36	0.59
1:A:469:LYS:O	1:A:473:GLU:HG3	2.02	0.58
1:B:377:HIS:HD2	2:B:1861:NBG:O6	1.86	0.58
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.85	0.58
1:A:286:PHE:CD1	1:A:385:GLU:HG3	2.38	0.58
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.84	0.58
1:A:152:LEU:HD22	1:A:827:VAL:HG12	1.85	0.58
1:A:629:VAL:HG11	1:A:750:PHE:HD1	1.67	0.58
1:A:66:ARG:HD3	1:A:236:ASN:HA	1.84	0.58
1:A:133:ASN:ND2	1:A:569:ARG:HH22	1.98	0.57
1:A:304:LEU:HD12	1:A:348:GLU:CG	2.34	0.57
1:B:64:VAL:HG23	1:B:65:GLY:N	2.18	0.57
1:A:727:GLU:HG3	1:A:729:LYS:HG2	1.86	0.57
1:A:689:ILE:HG23	1:A:689:ILE:O	2.05	0.57
1:B:66:ARG:HD3	1:B:236:ASN:HA	1.86	0.57
1:A:693:ASP:O	1:A:696:ASN:HB2	2.05	0.57
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.87	0.57
1:A:793:ASN:C	1:A:793:ASN:HD22	2.06	0.56
1:B:286:PHE:CD1	1:B:385:GLU:HG3	2.40	0.56
1:B:93:ARG:HG2	1:B:126:GLU:HG2	1.87	0.56
1:B:274:ASN:ND2	1:B:277:ARG:HH21	2.02	0.56
1:B:152:LEU:HD22	1:B:827:VAL:HG12	1.87	0.56
1:A:790:LEU:HG	1:A:797:TRP:CD1	2.41	0.56
1:B:693:ASP:O	1:B:696:ASN:HB2	2.05	0.56
1:B:656:VAL:O	1:B:660:THR:HG23	2.06	0.56
1:B:629:VAL:HG11	1:B:750:PHE:HD1	1.67	0.56
1:B:26:GLU:O	1:B:29:LYS:HG2	2.06	0.56
1:A:210:ASN:N	1:A:210:ASN:ND2	2.54	0.56
1:A:93:ARG:HG2	1:A:126:GLU:HG2	1.88	0.56
1:A:423:ASP:O	1:A:427:ARG:HB2	2.06	0.55
1:A:169:LYS:HE2	1:A:178:GLU:OE2	2.06	0.55
1:B:629:VAL:HG11	1:B:750:PHE:CE1	2.42	0.55
1:A:292:ARG:O	1:A:296:GLU:HG3	2.05	0.55
1:A:168:GLN:NE2	1:A:647:ASN:H	2.02	0.55
1:B:790:LEU:HG	1:B:797:TRP:CD1	2.41	0.55
1:B:793:ASN:C	1:B:793:ASN:HD22	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:O	1:B:296:GLU:HG3	2.06	0.55
1:B:423:ASP:O	1:B:427:ARG:HB2	2.05	0.55
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.89	0.55
1:A:29:LYS:HD3	6:A:2662:HOH:O	2.06	0.55
1:A:493:LEU:HD21	1:A:512:VAL:HG12	1.87	0.55
1:B:324:THR:HA	1:B:327:ASP:OD2	2.07	0.55
1:B:493:LEU:HD21	1:B:512:VAL:HG12	1.88	0.55
1:A:324:THR:HA	1:A:327:ASP:OD2	2.07	0.55
1:A:26:GLU:O	1:A:29:LYS:HG2	2.07	0.54
1:A:395:LEU:HB3	1:A:396:LEU:HD22	1.89	0.54
1:A:274:ASN:HD22	1:A:277:ARG:HE	1.54	0.54
1:A:630:VAL:HG21	1:A:642:VAL:CG2	2.38	0.54
1:A:629:VAL:HG11	1:A:750:PHE:CE1	2.42	0.54
1:B:169:LYS:HE2	1:B:178:GLU:OE2	2.08	0.54
1:B:630:VAL:HG21	1:B:642:VAL:CG2	2.37	0.54
1:B:571:HIS:H	1:B:576:GLN:HE22	1.56	0.54
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.90	0.54
1:B:184:ARG:NH2	6:B:2327:HOH:O	2.39	0.54
1:B:649:ARG:HB2	6:B:2534:HOH:O	2.06	0.54
1:A:678:ASN:ND2	1:A:679:MET:N	2.55	0.54
1:B:395:LEU:HB3	1:B:396:LEU:HD22	1.89	0.54
1:A:415:VAL:HG13	1:A:425:LEU:HD21	1.90	0.54
1:B:759:LYS:HE3	6:B:2657:HOH:O	2.08	0.54
1:A:237:THR:HB	6:A:2677:HOH:O	2.07	0.54
1:B:304:LEU:HD12	1:B:348:GLU:CG	2.37	0.54
1:B:211:THR:HB	6:B:2598:HOH:O	2.06	0.54
1:A:377:HIS:HD2	2:A:861:NBG:O6	1.92	0.53
1:B:274:ASN:HD22	1:B:277:ARG:HE	1.54	0.53
1:B:36:HIS:HD2	6:B:2279:HOH:O	1.92	0.53
1:B:689:ILE:HG23	1:B:689:ILE:O	2.09	0.53
1:B:435:GLY:O	1:B:436:SER:HB2	2.08	0.53
1:B:558:ASN:HB3	1:B:561:SER:HB3	1.90	0.53
1:B:571:HIS:HB2	6:B:2260:HOH:O	2.06	0.53
1:B:790:LEU:HG	1:B:797:TRP:HD1	1.74	0.53
1:A:554:LYS:HE2	1:A:554:LYS:O	2.09	0.53
1:B:554:LYS:O	1:B:554:LYS:HE2	2.09	0.53
1:B:573:TYR:HE1	1:B:672:GLU:HG2	1.74	0.53
1:A:571:HIS:H	1:A:576:GLN:HE22	1.56	0.53
1:B:527:ASP:O	1:B:531:LEU:HD23	2.08	0.53
1:B:380:LEU:HD22	1:B:380:LEU:H	1.73	0.53
1:B:415:VAL:HG13	1:B:425:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLY:O	1:A:436:SER:HB2	2.08	0.52
1:B:521:LEU:HB3	1:B:802:LEU:HD11	1.91	0.52
1:B:309:ARG:NH1	6:B:2239:HOH:O	2.42	0.52
1:B:216:ILE:HA	6:B:2337:HOH:O	2.09	0.52
1:A:573:TYR:HE1	1:A:672:GLU:HG2	1.73	0.52
1:B:678:ASN:ND2	1:B:679:MET:N	2.53	0.52
1:A:492:LEU:CD1	1:A:493:LEU:HD23	2.40	0.52
1:A:777:TYR:O	1:A:781:VAL:HG23	2.09	0.52
1:A:558:ASN:HB3	1:A:561:SER:HB3	1.91	0.52
1:B:661:ASP:HB3	1:B:797:TRP:CH2	2.44	0.52
1:A:656:VAL:O	1:A:660:THR:HG23	2.10	0.52
1:B:162:GLU:HG3	6:B:2126:HOH:O	2.08	0.52
1:A:29:LYS:HG3	1:A:33:ARG:NH1	2.25	0.52
1:A:235:ASN:CG	1:A:237:THR:HG23	2.31	0.52
1:A:170:ILE:C	1:A:171:ARG:HD2	2.31	0.52
1:A:304:LEU:HD12	1:A:348:GLU:HG3	1.92	0.52
1:B:605:ILE:O	1:B:644:PHE:HA	2.10	0.52
1:A:790:LEU:HG	1:A:797:TRP:HD1	1.74	0.51
1:B:605:ILE:HG21	1:B:623:ILE:HD13	1.91	0.51
1:A:420:LYS:N	1:A:420:LYS:HD2	2.25	0.51
1:B:133:ASN:ND2	1:B:569:ARG:NH2	2.41	0.51
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.91	0.51
1:B:777:TYR:O	1:B:781:VAL:HG23	2.10	0.51
1:A:678:ASN:HD22	1:A:678:ASN:N	2.08	0.51
1:A:687:LEU:HD12	1:A:797:TRP:CE2	2.46	0.51
1:B:235:ASN:CG	1:B:237:THR:HG23	2.31	0.51
1:B:380:LEU:HB3	1:B:382:GLU:OE1	2.10	0.51
1:B:168:GLN:NE2	1:B:647:ASN:H	2.03	0.51
1:B:29:LYS:HG3	1:B:33:ARG:NH1	2.26	0.51
1:B:492:LEU:CD1	1:B:493:LEU:HD23	2.40	0.51
1:A:527:ASP:O	1:A:531:LEU:HD23	2.11	0.51
1:A:521:LEU:HB3	1:A:802:LEU:HD11	1.92	0.51
1:A:24:VAL:O	1:A:28:LYS:HG3	2.11	0.51
1:A:543:LEU:O	1:A:547:GLN:HG3	2.11	0.50
1:A:419:PRO:HB2	1:A:420:LYS:HD2	1.93	0.50
1:B:106:ASN:HB3	6:B:2323:HOH:O	2.11	0.50
1:B:420:LYS:HD2	1:B:420:LYS:N	2.27	0.50
1:A:235:ASN:O	1:A:236:ASN:HB2	2.12	0.50
1:A:661:ASP:HB3	1:A:797:TRP:CH2	2.47	0.50
1:B:419:PRO:HB2	1:B:420:LYS:HD2	1.92	0.50
1:A:380:LEU:H	1:A:380:LEU:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:GLN:CA	1:A:789:GLN:HE21	2.04	0.50
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.12	0.50
1:B:380:LEU:N	1:B:380:LEU:HD22	2.27	0.50
1:A:433:GLU:HB3	1:A:437:LYS:HD2	1.93	0.50
1:B:678:ASN:HD22	1:B:678:ASN:N	2.09	0.49
1:A:296:GLU:OE2	1:A:385:GLU:OE1	2.29	0.49
1:A:678:ASN:ND2	1:A:679:MET:HG3	2.27	0.49
1:B:284:ASN:ND2	6:B:2008:HOH:O	2.44	0.49
1:A:661:ASP:O	1:A:797:TRP:HH2	1.95	0.49
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.49
1:A:763:ASN:HB2	6:A:2649:HOH:O	2.11	0.49
1:B:543:LEU:O	1:B:547:GLN:HG3	2.13	0.49
1:B:433:GLU:HB3	1:B:437:LYS:HD2	1.94	0.49
1:A:431:ILE:N	1:A:431:ILE:HD12	2.27	0.49
1:B:687:LEU:HD12	1:B:797:TRP:CE2	2.48	0.49
1:A:566:GLN:NE2	1:A:576:GLN:HA	2.26	0.49
1:A:626:VAL:O	1:A:630:VAL:HG13	2.13	0.49
1:A:133:ASN:ND2	1:A:281:PRO:HA	2.13	0.49
1:B:488:PRO:O	1:B:492:LEU:HB3	2.12	0.49
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.94	0.49
1:B:67:TRP:HA	1:B:238:VAL:HB	1.95	0.49
1:B:170:ILE:C	1:B:171:ARG:HD2	2.32	0.49
1:A:64:VAL:HG21	1:B:37:PHE:CD1	2.47	0.49
1:A:64:VAL:HG23	1:A:65:GLY:H	1.76	0.49
1:A:23:ASN:HD21	1:A:26:GLU:HG2	1.77	0.49
1:A:380:LEU:HB3	1:A:382:GLU:OE1	2.12	0.49
1:B:399:HIS:HD2	6:B:2009:HOH:O	1.96	0.49
1:B:304:LEU:HD12	1:B:348:GLU:HG3	1.95	0.49
1:A:605:ILE:HG21	1:A:623:ILE:HD13	1.93	0.49
1:B:431:ILE:HD12	1:B:431:ILE:N	2.28	0.48
1:B:275:ILE:O	1:B:295:GLN:HG2	2.13	0.48
1:A:630:VAL:O	1:A:636:VAL:HG21	2.13	0.48
1:B:571:HIS:CD2	6:B:2260:HOH:O	2.65	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.96	0.48
1:B:23:ASN:HD21	1:B:26:GLU:HG2	1.78	0.48
1:A:29:LYS:HE2	1:A:33:ARG:HH12	1.74	0.48
1:B:630:VAL:O	1:B:636:VAL:HG21	2.13	0.48
1:B:483:THR:O	1:B:815:ARG:NH2	2.41	0.48
1:B:767:TYR:HB2	1:B:768:HIS:CE1	2.49	0.48
1:A:22:GLU:HG3	6:A:2290:HOH:O	2.13	0.48
1:A:504:ALA:HB1	6:A:2617:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:O	1:B:28:LYS:HG3	2.14	0.48
1:B:109:ASP:OD1	1:B:119:ILE:HD13	2.14	0.48
1:A:566:GLN:HA	6:A:2231:HOH:O	2.12	0.48
1:B:286:PHE:CE1	1:B:385:GLU:HG3	2.49	0.48
1:A:380:LEU:N	1:A:380:LEU:HD22	2.29	0.48
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.95	0.48
1:A:767:TYR:HB2	1:A:768:HIS:CE1	2.49	0.48
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.95	0.47
1:A:286:PHE:CE1	1:A:385:GLU:HG3	2.49	0.47
1:B:235:ASN:O	1:B:236:ASN:HB2	2.13	0.47
1:B:64:VAL:HG23	1:B:65:GLY:H	1.78	0.47
1:A:450:HIS:HE1	6:A:2171:HOH:O	1.96	0.47
1:A:709:PHE:HB3	1:A:783:CYS:SG	2.54	0.47
1:B:678:ASN:ND2	1:B:679:MET:HG3	2.29	0.47
1:B:661:ASP:O	1:B:797:TRP:HH2	1.96	0.47
1:B:626:VAL:O	1:B:630:VAL:HG13	2.14	0.47
1:B:171:ARG:HH11	1:B:171:ARG:HG2	1.79	0.47
1:B:216:ILE:HB	6:B:2373:HOH:O	2.15	0.47
1:A:389:VAL:HG11	1:A:404:TYR:OH	2.15	0.47
1:A:754:GLN:NE2	1:A:757:LEU:HD13	2.30	0.47
1:A:136:LEU:C	1:A:136:LEU:HD23	2.35	0.47
1:A:174:TRP:CD2	1:A:621:LYS:HG3	2.50	0.47
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.97	0.47
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.47
1:B:424:ARG:HD2	1:B:428:MET:SD	2.54	0.47
1:B:754:GLN:NE2	1:B:757:LEU:HD13	2.30	0.47
1:A:561:SER:HB2	1:A:601:ARG:HA	1.96	0.47
1:A:72:GLN:HE21	1:A:76:ASP:CG	2.18	0.47
1:B:455:VAL:H	1:B:459:HIS:CD2	2.31	0.47
1:A:628:ASP:O	1:A:632:ASN:ND2	2.48	0.47
1:B:389:VAL:HG11	1:B:404:TYR:OH	2.15	0.47
1:B:517:GLN:OE1	1:B:520:LYS:HE3	2.15	0.46
1:A:630:VAL:HG23	1:A:631:ASN:N	2.30	0.46
1:B:235:ASN:ND2	1:B:237:THR:H	2.13	0.46
1:A:791:TYR:HA	1:A:797:TRP:CD1	2.51	0.46
1:B:697:VAL:O	1:B:701:GLU:HG3	2.15	0.46
1:B:507:ILE:HG13	6:B:2377:HOH:O	2.14	0.46
1:B:561:SER:HB2	1:B:601:ARG:HA	1.96	0.46
1:A:83:TYR:HE1	1:A:310:ARG:HH21	1.62	0.46
1:B:91:MET:HB2	1:B:129:ALA:HB3	1.96	0.46
1:A:569:ARG:O	1:A:574:LYS:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:ASP:O	1:A:789:GLN:HG2	2.16	0.46
1:B:110:GLU:HB2	6:B:2222:HOH:O	2.14	0.46
1:A:697:VAL:O	1:A:701:GLU:HG3	2.16	0.46
1:B:72:GLN:HE21	1:B:76:ASP:CG	2.19	0.46
1:B:791:TYR:HA	1:B:797:TRP:CD1	2.51	0.46
1:A:37:PHE:CD1	1:B:64:VAL:HG21	2.51	0.46
1:A:746:ASP:OD2	1:A:762:ILE:HG21	2.16	0.46
1:B:566:GLN:NE2	1:B:576:GLN:HA	2.28	0.45
1:B:764:MET:CE	1:B:765:LEU:HD13	2.46	0.45
1:B:579:ASN:HD22	1:B:579:ASN:C	2.19	0.45
1:B:422:VAL:HG23	1:B:423:ASP:N	2.31	0.45
1:A:424:ARG:HD2	1:A:428:MET:SD	2.56	0.45
1:B:630:VAL:HG23	1:B:631:ASN:N	2.30	0.45
1:A:483:THR:O	1:A:815:ARG:NH2	2.46	0.45
1:B:527:ASP:O	1:B:531:LEU:CD2	2.65	0.45
1:A:492:LEU:HD13	1:A:500:ALA:HB2	1.98	0.45
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.16	0.45
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.99	0.45
1:B:569:ARG:O	1:B:574:LYS:HD2	2.16	0.45
1:B:296:GLU:OE2	1:B:385:GLU:OE1	2.35	0.45
1:A:399:HIS:HD2	6:A:2119:HOH:O	2.00	0.45
1:A:536:LYS:O	1:A:540:GLU:HG3	2.17	0.45
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.57	0.45
1:A:133:ASN:ND2	1:A:569:ARG:NH2	2.45	0.45
1:B:210:ASN:ND2	1:B:210:ASN:N	2.52	0.45
1:B:174:TRP:CD2	1:B:621:LYS:HG3	2.52	0.45
1:A:235:ASN:ND2	1:A:237:THR:H	2.15	0.45
1:A:793:ASN:C	1:A:793:ASN:ND2	2.70	0.45
1:A:435:GLY:O	1:A:436:SER:CB	2.64	0.45
1:B:827:VAL:CG1	1:B:828:GLU:N	2.79	0.45
1:B:402:ILE:O	1:B:406:ILE:HG13	2.17	0.45
1:A:133:ASN:HD21	1:A:281:PRO:CA	2.16	0.44
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.99	0.44
1:A:422:VAL:HG23	1:A:423:ASP:N	2.31	0.44
1:A:645:LEU:HD22	1:A:652:LEU:HD11	2.00	0.44
1:B:628:ASP:O	1:B:632:ASN:ND2	2.51	0.44
1:B:678:ASN:ND2	1:B:678:ASN:N	2.66	0.44
1:B:330:PRO:HB3	1:B:370:LYS:HB3	1.99	0.44
1:A:636:VAL:HG23	1:A:637:GLY:N	2.32	0.44
1:B:396:LEU:HB3	1:B:399:HIS:CD2	2.53	0.44
1:A:196:PHE:HD1	1:A:309:ARG:HH11	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:GLY:O	1:B:710:ILE:HA	2.18	0.44
1:B:336:GLN:OE1	1:B:373:ALA:HB3	2.17	0.44
1:A:402:ILE:O	1:A:406:ILE:HG13	2.18	0.44
1:B:143:PHE:CG	1:B:817:ILE:HD11	2.53	0.44
1:A:143:PHE:CG	1:A:817:ILE:HD11	2.52	0.44
1:B:112:ILE:HG23	1:B:117:LEU:HB2	1.99	0.44
1:A:275:ILE:O	1:A:295:GLN:HG2	2.17	0.44
1:B:136:LEU:HD23	1:B:136:LEU:C	2.38	0.44
1:B:569:ARG:HD2	1:B:608:LYS:O	2.17	0.44
1:A:678:ASN:N	1:A:678:ASN:ND2	2.66	0.44
1:B:43:ARG:NH2	1:B:115:LEU:HB3	2.32	0.44
1:A:325:VAL:HG23	1:A:326:PHE:CD1	2.52	0.44
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.00	0.44
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.99	0.44
1:A:274:ASN:ND2	1:A:277:ARG:HE	2.15	0.43
1:A:171:ARG:HH11	1:A:171:ARG:HG2	1.83	0.43
1:A:396:LEU:HB3	1:A:399:HIS:CD2	2.53	0.43
1:B:196:PHE:HD1	1:B:309:ARG:HH11	1.66	0.43
1:B:510:ASP:HB2	6:B:2665:HOH:O	2.17	0.43
1:B:435:GLY:O	1:B:436:SER:CB	2.66	0.43
1:B:143:PHE:O	1:B:147:MET:HG3	2.18	0.43
1:A:735:LEU:HA	1:A:736:PRO:HD2	1.87	0.43
1:A:23:ASN:HD21	1:A:26:GLU:CG	2.31	0.43
1:A:660:THR:HG1	1:A:681:PHE:HD2	1.61	0.43
1:A:827:VAL:CG1	1:A:828:GLU:N	2.81	0.43
1:B:565:VAL:HG11	1:B:660:THR:HG22	1.99	0.43
1:B:492:LEU:HD13	1:B:500:ALA:HB2	1.99	0.43
1:B:492:LEU:HD12	1:B:493:LEU:HD23	2.00	0.43
1:A:455:VAL:H	1:A:459:HIS:CD2	2.32	0.43
1:A:527:ASP:O	1:A:531:LEU:CD2	2.66	0.43
1:A:568:LYS:O	1:A:607:GLY:HA3	2.17	0.43
1:B:29:LYS:HE2	1:B:33:ARG:HH12	1.77	0.43
1:B:746:ASP:OD2	1:B:762:ILE:HG21	2.18	0.43
1:B:83:TYR:HE1	1:B:310:ARG:HH21	1.64	0.43
1:A:43:ARG:NH2	1:A:115:LEU:HB3	2.34	0.43
1:A:764:MET:CE	1:A:765:LEU:HD13	2.48	0.43
1:B:662:LEU:CD2	1:B:689:ILE:HG22	2.47	0.43
1:B:235:ASN:ND2	1:B:237:THR:HG23	2.34	0.43
1:A:36:HIS:HD2	6:A:2604:HOH:O	2.00	0.43
1:A:579:ASN:C	1:A:579:ASN:HD22	2.20	0.43
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:ND2	1:B:277:ARG:HE	2.14	0.43
1:B:636:VAL:HG23	1:B:637:GLY:N	2.33	0.43
1:B:713:MET:HB3	1:B:717:ASP:HB2	2.00	0.43
1:A:510:ASP:HB2	6:A:2379:HOH:O	2.19	0.43
1:A:346:ILE:HD13	1:A:448:GLY:HA3	2.00	0.43
1:A:598:PHE:HE1	6:A:2544:HOH:O	2.00	0.43
1:A:577:LEU:HB2	6:A:2145:HOH:O	2.19	0.43
1:B:163:TYR:HB2	1:B:278:VAL:HG13	2.01	0.42
1:B:568:LYS:O	1:B:607:GLY:HA3	2.19	0.42
1:A:386:ARG:HA	1:A:439:ILE:O	2.19	0.42
1:B:793:ASN:ND2	1:B:793:ASN:C	2.72	0.42
1:A:102:LEU:O	1:A:104:LEU:HD13	2.19	0.42
1:B:726:TYR:OH	1:B:774:PHE:HB2	2.19	0.42
1:A:569:ARG:HD2	1:A:608:LYS:O	2.19	0.42
1:A:492:LEU:HD12	1:A:493:LEU:HD23	2.01	0.42
1:B:536:LYS:O	1:B:540:GLU:HG3	2.19	0.42
1:A:731:TYR:HB3	1:A:735:LEU:HD12	2.00	0.42
1:B:74:TYR:CZ	1:B:153:ALA:HA	2.54	0.42
1:B:698:GLU:O	1:B:702:GLU:HG2	2.19	0.42
1:B:735:LEU:HA	1:B:736:PRO:HD2	1.87	0.42
1:A:163:TYR:HB2	1:A:278:VAL:HG13	2.00	0.42
1:B:626:VAL:O	1:B:629:VAL:HG13	2.19	0.42
1:B:43:ARG:HD2	1:B:51:TYR:OH	2.20	0.42
1:B:731:TYR:HB3	1:B:735:LEU:HD12	2.02	0.42
1:B:630:VAL:CG2	1:B:631:ASN:N	2.83	0.42
1:B:100:ILE:HD12	1:B:494:LEU:HD23	2.02	0.42
1:B:619:ILE:O	1:B:623:ILE:HG13	2.20	0.42
1:B:754:GLN:N	1:B:755:PRO:HD3	2.33	0.42
1:A:764:MET:SD	1:A:764:MET:C	2.99	0.42
1:B:133:ASN:HD21	1:B:281:PRO:CA	2.16	0.42
1:A:690:GLY:O	1:A:710:ILE:HA	2.19	0.42
1:B:415:VAL:HG23	1:B:416:ALA:N	2.35	0.41
1:B:300:VAL:HG13	1:B:345:ALA:HA	2.02	0.41
1:A:100:ILE:HD12	1:A:494:LEU:CD2	2.50	0.41
1:B:379:VAL:HG21	1:B:670:GLY:O	2.20	0.41
1:B:407:ASN:ND2	1:B:431:ILE:HD13	2.35	0.41
1:A:225:PRO:HD3	1:A:244:TRP:CZ3	2.56	0.41
1:B:720:ALA:O	1:B:723:LYS:HB3	2.21	0.41
1:B:225:PRO:HD3	1:B:244:TRP:CZ3	2.55	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.35	0.41
1:B:574:LYS:NZ	1:B:672:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:ND2	1:A:237:THR:HG23	2.36	0.41
1:B:304:LEU:O	1:B:308:ILE:HG12	2.20	0.41
1:B:712:GLY:HA2	6:B:2606:HOH:O	2.20	0.41
1:A:378:THR:HA	6:A:2334:HOH:O	2.19	0.41
1:A:206:VAL:HG23	1:A:397:PRO:HB2	2.02	0.41
1:A:517:GLN:OE1	1:A:520:LYS:HE3	2.21	0.41
1:A:565:VAL:HG11	1:A:660:THR:HG22	2.02	0.41
1:B:237:THR:HB	6:B:2143:HOH:O	2.19	0.41
1:B:395:LEU:O	1:B:396:LEU:HD13	2.21	0.41
1:B:396:LEU:N	1:B:396:LEU:HD22	2.36	0.41
1:B:339:ASP:O	1:B:342:PRO:HD2	2.21	0.41
1:A:415:VAL:HG23	1:A:416:ALA:N	2.34	0.41
1:B:174:TRP:CZ2	1:B:621:LYS:HG3	2.56	0.41
1:A:395:LEU:O	1:A:396:LEU:HD13	2.21	0.41
1:B:542:LYS:NZ	6:B:2703:HOH:O	2.53	0.41
1:B:386:ARG:HA	1:B:439:ILE:O	2.20	0.41
1:B:325:VAL:HG23	1:B:326:PHE:CD1	2.56	0.41
1:B:785:ASP:O	1:B:789:GLN:HG2	2.20	0.41
1:A:630:VAL:CG2	1:A:631:ASN:N	2.83	0.41
1:A:407:ASN:ND2	1:A:431:ILE:HD13	2.36	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.21	0.41
1:B:193:ARG:HB2	1:B:225:PRO:HG2	2.02	0.41
1:B:545:PHE:O	1:B:548:PHE:HB3	2.20	0.41
1:B:42:ASP:HB2	6:B:2717:HOH:O	2.21	0.41
1:B:100:ILE:HD12	1:B:494:LEU:CD2	2.50	0.41
1:A:626:VAL:O	1:A:629:VAL:HG13	2.21	0.41
1:A:355:ASP:HA	6:A:2399:HOH:O	2.19	0.41
1:A:66:ARG:HD2	1:A:236:ASN:HA	2.00	0.41
1:B:615:MET:O	1:B:619:ILE:HG13	2.21	0.41
1:B:410:HIS:O	1:B:414:ILE:HD13	2.21	0.41
1:A:423:ASP:OD2	1:A:426:ARG:NE	2.47	0.40
1:B:662:LEU:C	1:B:662:LEU:CD2	2.87	0.40
1:A:330:PRO:HB3	1:A:370:LYS:HB3	2.03	0.40
1:A:415:VAL:CG1	1:A:425:LEU:HD11	2.48	0.40
1:B:214:LYS:HA	6:B:2706:HOH:O	2.21	0.40
1:A:574:LYS:NZ	1:A:672:GLU:OE2	2.53	0.40
1:B:415:VAL:CG1	1:B:425:LEU:HD11	2.48	0.40
1:B:36:HIS:O	1:B:40:VAL:HA	2.22	0.40
1:A:109:ASP:CB	6:A:2581:HOH:O	2.57	0.40
1:B:687:LEU:HA	1:B:687:LEU:HD23	1.92	0.40
1:B:458:ILE:HG23	1:B:459:HIS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:TYR:OH	1:B:291:LEU:HB3	2.22	0.40
1:A:161:TYR:HA	1:A:276:SER:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLU:OE1	1:B:312:LYS:NZ[2_555]	2.03	0.17
1:A:210:ASN:OD1	6:B:2026:HOH:O[2_665]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/847 (92%)	737 (95%)	39 (5%)	3 (0%)	39	42
1	B	779/847 (92%)	733 (94%)	44 (6%)	2 (0%)	46	50
All	All	1558/1694 (92%)	1470 (94%)	83 (5%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	SER
1	B	436	SER
1	A	435	GLY
1	B	435	GLY
1	A	342	PRO

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	688/740 (93%)	647 (94%)	41 (6%)	24	26
1	B	688/740 (93%)	645 (94%)	43 (6%)	22	24
All	All	1376/1480 (93%)	1292 (94%)	84 (6%)	23	26

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	90	TYR
1	A	95	LEU
1	A	102	LEU
1	A	128	ASP
1	A	171	ARG
1	A	210	ASN
1	A	235	ASN
1	A	237	THR
1	A	243	LEU
1	A	247	ARG
1	A	278	VAL
1	A	325	VAL
1	A	361	TRP
1	A	379	VAL
1	A	433	GLU
1	A	466	LYS
1	A	490	ARG
1	A	499	LEU
1	A	502	LEU
1	A	539	GLN
1	A	554	LYS
1	A	568	LYS
1	A	573	TYR
1	A	576	GLN
1	A	577	LEU
1	A	579	ASN
1	A	613	TYR
1	A	622	LEU
1	A	629	VAL
1	A	645	LEU

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Mol	Chain	Res	Type
1	A	652	LEU
1	A	678	ASN
1	A	683	LEU
1	A	708	LEU
1	A	730	GLU
1	A	733	GLU
1	A	789	GLN
1	A	793	ASN
1	A	797	TRP
1	A	815	ARG
1	B	43	ARG
1	B	90	TYR
1	B	95	LEU
1	B	102	LEU
1	B	128	ASP
1	B	171	ARG
1	B	210	ASN
1	B	235	ASN
1	B	237	THR
1	B	243	LEU
1	B	247	ARG
1	B	278	VAL
1	B	325	VAL
1	B	361	TRP
1	B	379	VAL
1	B	433	GLU
1	B	466	LYS
1	B	490	ARG
1	B	494	LEU
1	B	499	LEU
1	B	502	LEU
1	B	539	GLN
1	B	554	LYS
1	B	568	LYS
1	B	573	TYR
1	B	576	GLN
1	B	577	LEU
1	B	579	ASN
1	B	613	TYR
1	B	622	LEU
1	B	629	VAL
1	B	645	LEU

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Mol	Chain	Res	Type
1	B	652	LEU
1	B	678	ASN
1	B	683	LEU
1	B	708	LEU
1	B	730	GLU
1	B	733	GLU
1	B	765	LEU
1	B	789	GLN
1	B	793	ASN
1	B	797	TRP
1	B	815	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	36	HIS
1	A	72	GLN
1	A	96	GLN
1	A	133	ASN
1	A	167	ASN
1	A	168	GLN
1	A	210	ASN
1	A	235	ASN
1	A	239	ASN
1	A	264	GLN
1	A	274	ASN
1	A	282	ASN
1	A	284	ASN
1	A	377	HIS
1	A	399	HIS
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	484	ASN
1	A	541	ASN
1	A	547	GLN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	678	ASN
1	A	754	GLN

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Mol	Chain	Res	Type
1	A	789	GLN
1	A	793	ASN
1	A	822	GLN
1	A	823	ASN
1	A	826	ASN
1	B	34	HIS
1	B	36	HIS
1	B	72	GLN
1	B	106	ASN
1	B	133	ASN
1	B	167	ASN
1	B	168	GLN
1	B	210	ASN
1	B	235	ASN
1	B	239	ASN
1	B	264	GLN
1	B	274	ASN
1	B	282	ASN
1	B	284	ASN
1	B	369	GLN
1	B	377	HIS
1	B	399	HIS
1	B	450	HIS
1	B	459	HIS
1	B	481	ASN
1	B	484	ASN
1	B	541	ASN
1	B	547	GLN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	678	ASN
1	B	754	GLN
1	B	789	GLN
1	B	793	ASN
1	B	822	GLN
1	B	826	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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	$\# Z  > 2$
4	PLP	A	860	1	15,15,16	1.56	2 (13%)	21,22,23	1.31	3 (14%)
2	NBG	A	861	-	15,15,15	1.54	3 (20%)	21,21,21	1.05	1 (4%)
3	CP4	A	862	-	33,37,37	1.80	10 (30%)	40,50,50	2.03	12 (30%)
4	PLP	B	1860	1	15,15,16	1.99	3 (20%)	21,22,23	1.43	2 (9%)
2	NBG	B	1861	-	15,15,15	1.64	3 (20%)	21,21,21	1.20	2 (9%)
5	MPD	B	1902	-	6,7,7	0.69	0	7,10,10	0.56	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
4	PLP	A	860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
3	CP4	A	862	-	-	0/15/21/21	0/4/4/4
4	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1
5	MPD	B	1902	-	1/1/2/2	0/5/5/5	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1860	PLP	C4A-C4	-6.05	1.39	1.51
4	A	860	PLP	C4A-C4	-4.34	1.42	1.51
3	A	862	CP4	C2-C6	-2.86	1.34	1.40
4	B	1860	PLP	C3-C2	-2.68	1.38	1.40
3	A	862	CP4	C26-C23	-2.15	1.36	1.40
4	A	860	PLP	P-O3P	-2.08	1.47	1.54
4	B	1860	PLP	C5A-C5	2.05	1.56	1.50
2	B	1861	NBG	C3-C2	2.09	1.57	1.52
2	A	861	NBG	C3-C2	2.26	1.58	1.52
2	A	861	NBG	C1-N1	2.64	1.46	1.43
3	A	862	CP4	C26-C28	2.66	1.51	1.41
3	A	862	CP4	C2-C0	2.68	1.51	1.41
3	A	862	CP4	C8-C7	2.91	1.43	1.38
3	A	862	CP4	C31-C32	3.11	1.44	1.38
3	A	862	CP4	C3-C7	3.21	1.43	1.36
3	A	862	CP4	C30-C32	3.24	1.43	1.36
2	B	1861	NBG	C2-C1	3.26	1.56	1.53
3	A	862	CP4	C29-C31	3.33	1.43	1.36
3	A	862	CP4	C5-C8	3.56	1.44	1.36
2	B	1861	NBG	C1-N1	3.89	1.47	1.43
2	A	861	NBG	C2-C1	4.16	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	862	CP4	C2-C0-C1	-4.19	102.62	106.27
3	A	862	CP4	C26-C28-C27	-3.90	102.87	106.27
3	A	862	CP4	C31-C29-C27	-3.43	117.15	120.88
3	A	862	CP4	C8-C5-C1	-3.37	117.22	120.88
4	B	1860	PLP	O4P-C5A-C5	-3.18	103.74	108.99
3	A	862	CP4	C32-C30-C28	-2.77	117.44	119.19
3	A	862	CP4	C7-C3-C0	-2.72	117.47	119.19
4	A	860	PLP	O4P-C5A-C5	-2.41	105.02	108.99
3	A	862	CP4	O24-C22-C23	-2.36	116.20	121.23
3	A	862	CP4	O12-C9-C6	-2.26	116.42	121.23
4	A	860	PLP	O2P-P-O4P	-2.21	100.19	106.56
2	B	1861	NBG	C2-C1-N1	-2.05	109.15	111.44
4	B	1860	PLP	O3P-P-O1P	2.15	117.50	110.58
4	A	860	PLP	O3P-P-O2P	2.46	116.75	107.38
2	B	1861	NBG	C5-O5-C1	3.36	117.38	112.49
2	A	861	NBG	C5-O5-C1	3.46	117.52	112.49
3	A	862	CP4	C23-N25-C27	3.61	111.92	104.47
3	A	862	CP4	C6-N4-C1	3.75	112.20	104.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	862	CP4	C6-C9-N11	4.20	121.07	115.42
3	A	862	CP4	C23-C22-N21	4.73	121.79	115.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1902	MPD	C4

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	861	NBG	1	0
2	B	1861	NBG	1	0

## 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 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.