



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 01:29 PM EDT

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-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

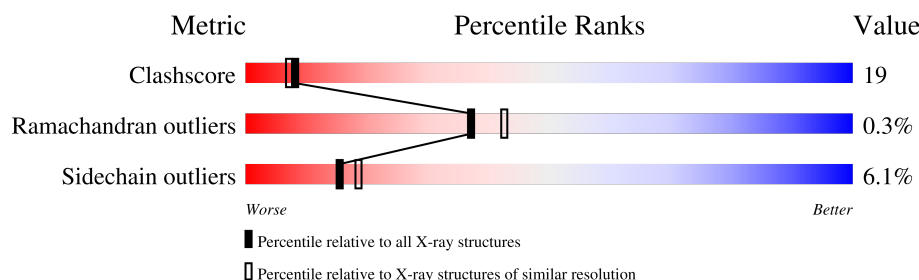
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	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.

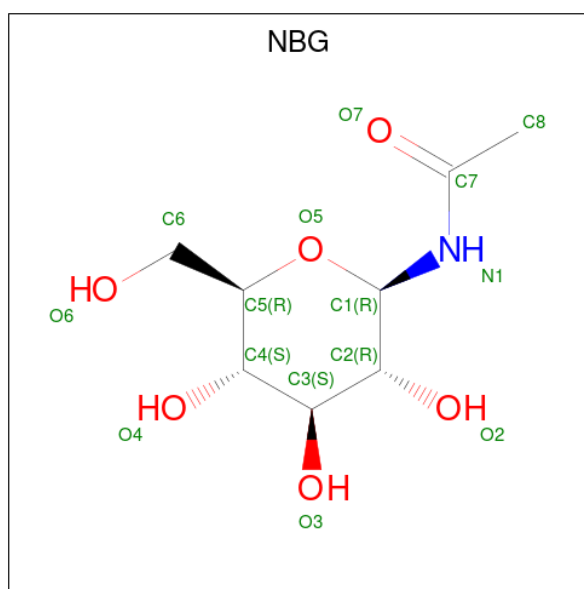
- Molecule 1 is a protein called LIVER GLYCOGEN PHOSPHORYLASE.

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 N-acetyl-beta-D-glucopyranosylamine (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



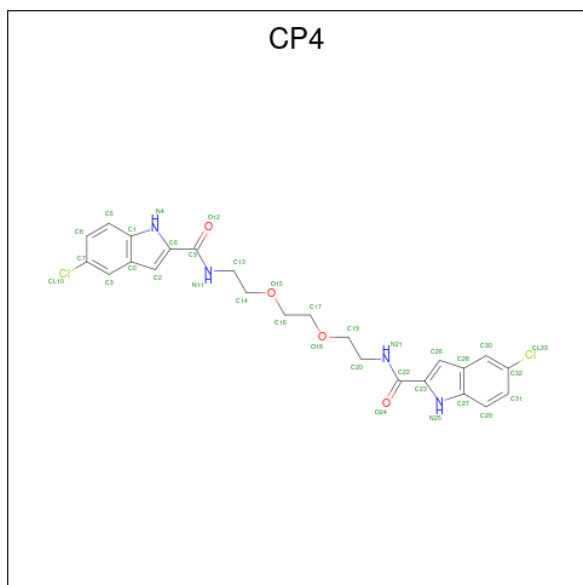
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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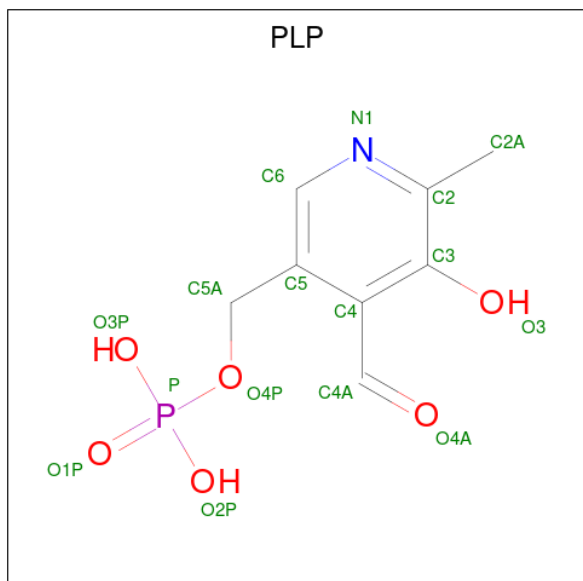
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is BIS[5-CHLORO-1H-INDOL-2-YL-CARBONYL-AMINOETHYL]-ETHYLEN E GLYCOL (three-letter code: CP4) (formula: $C_{24}H_{24}Cl_2N_4O_4$).



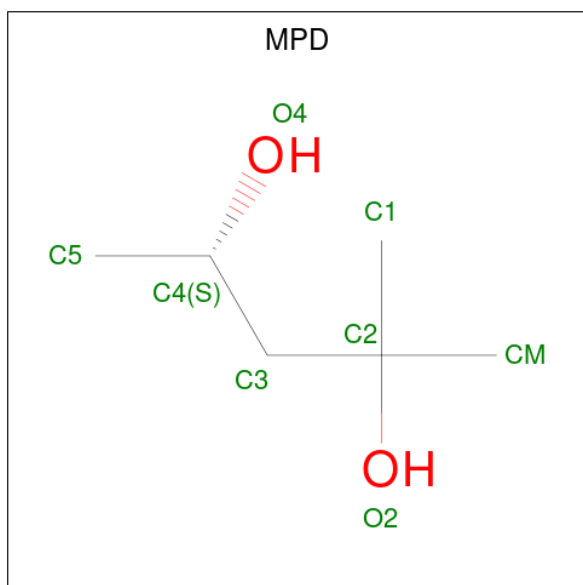
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			34	24	2	4	4	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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: C₆H₁₄O₂).



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	V565	E473	E382	R292	D181	R81
SER	F736	Q566	E473	E382	R292	D181	V82
ASN		Q567	T483	E385	Q295	R184	Y83
GLU	V656	F567	T483	R386	E296		Y90
SER	I657	R569	P488	V359		R193	M91
ASN	P658	I570	R489	V359		F196	G92
LYS	A659	H571	R490	L395	L304		R93
VAL	T660	S572	R490	L396		N210	I94
ASN	D661	Y573	L492	P397	I308	T211	Q96
GLY	P755	K574	L493	R398	R309		
ASN	D756	R575	L493	H399	R310		
ASN	L757	Q576	L494		F311	K214	I100
	F758	L577		I402	R312	W215	M101
	K759	S578	L499	I403	A313	L216	L102
	I762	C580	A500	Y404	S314		
			E501	E405	LYS	P225	N106
	N763	F594	L502	I406	PHE		
N764	M678	LYS	E505	N407	GLY	N235	D109
L765	M679	LYS	K506	Q408	GLY	N236	E110
F766	K680	LEU	I507	K409	THR	A111	
Y767	F681	F598	G508	H410	ARG	V238	I112
H768	M682		E509		GLY		
	L683	R601	D510	I414	ALA	L243	L115
F774			Y511	V415	GLY	W244	G116
	L687	I605	V512	A416			L117
Y777	T688	G606	Q517	P419	R247	R247	D118
	G689	G607		K420	F326	A248	I119
V781	K682	K608	K520	D421	P249	ASN	E126
C783	D693		L521	V422	A328	ASP	E127
G784		Y613	F524	D423	F329	PHE	D128
D785	N696	H614		R424	P330	ASN	A129
K786	V697	M615	D627	L425	Q336	LEU	
V787	E698			R426		ARG	N133
S788		I619	L531	R427	D339	ASP	
Q789	E701	I620		M428		PHE	L136
L790	E702	K621	K536	I431	P342	ASN	F143
Y791		L622	Q539	E432	A345	VAL	
F792	L708	I623	E540	E433	I346	D261	M147
N793	F709		N541	E434	P347	Y262	
W797	I710	V626	K542	G435	E348	I263	L152
	G712	D628	L543	S436			A153
L802	M713	W629	L543	K437	D355	N270	A154
		V630	F544	R438			Y155
R810	D717	N631	F545	I439	W361	N274	R160
	A720	N632	S546			I275	Y161
R815		D633	Q547	G448	E366	S276	E162
T816	A723		F548	S449	L367	R277	Y163
I817		V636		H450		L279	
	K723	Q637	T551		K370		
			K554	V455	A373	Y280	Q168
W827	Y726	V642	V555			P281	K169
E828	E727	I643		I458	H377	N284	I170
P829	A728	F644	N558	H459	T378	F285	R171
S830	K729	L645			V379	P286	
	E730	E646	S561	K466	L380		W174
ASP	Y731	M647					
LEU	Y732	Y648		K469			
LYS	E733						
ILE							
SER	A734	R649					E178

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	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	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 ²)	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: PLP, CP4, MPD, 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	0.35	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:HE21	1:B:789:GLN:HA	1.24	1.02
1:A:133:ASN:HD22	1:A:569:ARG:NH2	1.60	1.00
1:A:789:GLN:HE21	1:A:789:GLN:HA	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:A:678:ASN:HD22	1:A:679:MET:H	1.25	0.84
1:B:163:TYR:CE1	1:B:181:ASP:HB3	2.12	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:163:TYR:HE1	1:B:181:ASP:HB3	1.52	0.71
1:B:678:ASN:HD22	1:B:679:MET:N	1.88	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:415:VAL:HG12	1:A:425:LEU:HD11	1.74	0.69
1:A:789:GLN:HA	1:A:789:GLN:NE2	2.04	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:580:CYS:SG	1:B:622:LEU:HD13	2.35	0.67
1:B:662:LEU:HD21	1:B:689:ILE:HG22	1.75	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:174:TRP:CE2	1:A:621:LYS:HG3	2.31	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: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:A:66:ARG:CD	1:A:236:ASN:HA	2.27	0.65
1:B:678:ASN:ND2	1:B:679:MET:H	1.93	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:A:450:HIS:HD2	6:A:2481:HOH:O	1.81	0.63
1:B:630:VAL:HG21	1:B:642:VAL:HG23	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:A:506:LYS:HD2	1:A:524:PHE:CE2	2.34	0.63
1:B:262:TYR:HD2	1:B:263:ILE:HD12	1.64	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:361:TRP:CZ3	1:A:409:LYS:HD3	2.36	0.61
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.81	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:310:ARG:HD3	6:B:2366:HOH:O	2.02	0.60
1:B:469:LYS:O	1:B:473:GLU:HG3	2.01	0.60
1:B:633:ASP:O	1:B:636:VAL:HG22	2.01	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:61:ASP:O	1:A:64:VAL:HG22	2.01	0.60
1:A:662:LEU:C	1:A:662:LEU:HD23	2.22	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:633:ASP:O	1:A:636:VAL:HG22	2.02	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:A:571:HIS:H	1:A:576:GLN:NE2	1.99	0.60
1:B:662:LEU:C	1:B:662:LEU:HD23	2.21	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:A:124:GLU:HG2	6:A:2701:HOH:O	2.02	0.59
1:B:727:GLU:HG3	1:B:729:LYS:HG2	1.84	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:286:PHE:CD1	1:A:385:GLU:HG3	2.38	0.58
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.85	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:66:ARG:HD3	1:A:236:ASN:HA	1.84	0.58
1:A:629:VAL:HG11	1:A:750:PHE:HD1	1.67	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:A:693:ASP:O	1:A:696:ASN:HB2	2.05	0.57
1:B:66:ARG:HD3	1:B:236:ASN:HA	1.86	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:93:ARG:HG2	1:B:126:GLU:HG2	1.87	0.56
1:B:286:PHE:CD1	1:B:385:GLU:HG3	2.40	0.56
1:B:152:LEU:HD22	1:B:827:VAL:HG12	1.87	0.56
1:B:274:ASN:ND2	1:B:277:ARG:HH21	2.02	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:93:ARG:HG2	1:A:126:GLU:HG2	1.88	0.56
1:A:210:ASN:N	1:A:210:ASN:ND2	2.54	0.56
1:A:169:LYS:HE2	1:A:178:GLU:OE2	2.06	0.55
1:A:423:ASP:O	1:A:427:ARG:HB2	2.06	0.55
1:A:292:ARG:O	1:A:296:GLU:HG3	2.05	0.55
1:B:629:VAL:HG11	1:B:750:PHE:CE1	2.42	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:160:ARG:HB2	1:B:243:LEU:HB3	1.89	0.55
1:B:423:ASP:O	1:B:427:ARG:HB2	2.05	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:A:324:THR:HA	1:A:327:ASP:OD2	2.07	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: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:629:VAL:HG11	1:A:750:PHE:CE1	2.42	0.54
1:A:630:VAL:HG21	1:A:642:VAL:CG2	2.38	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: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:571:HIS:H	1:B:576:GLN:HE22	1.56	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:A:237:THR:HB	6:A:2677:HOH:O	2.07	0.54
1:B:211:THR:HB	6:B:2598:HOH:O	2.06	0.54
1:B:304:LEU:HD12	1:B:348:GLU:CG	2.37	0.54
1:B:759:LYS:HE3	6:B:2657:HOH:O	2.08	0.54
1:A:377:HIS:HD2	2:A:861:NBG:O6	1.92	0.53
1:B:36:HIS:HD2	6:B:2279:HOH:O	1.92	0.53
1:B:274:ASN:HD22	1:B:277:ARG:HE	1.54	0.53
1:B:689:ILE:O	1:B:689:ILE:HG23	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:A:554:LYS:HE2	1:A:554:LYS:O	2.09	0.53
1:B:554:LYS:HE2	1:B:554:LYS:O	2.09	0.53
1:B:790:LEU:HG	1:B:797:TRP:HD1	1.74	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:H	1:B:380:LEU:HD22	1.73	0.53
1:A:435:GLY:O	1:A:436:SER:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HG13	1:B:425:LEU:HD21	1.90	0.52
1:B:521:LEU:HB3	1:B:802:LEU:HD11	1.91	0.52
1:B:216:ILE:HA	6:B:2337:HOH:O	2.09	0.52
1:B:309:ARG:NH1	6:B:2239:HOH:O	2.42	0.52
1:A:492:LEU:CD1	1:A:493:LEU:HD23	2.40	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:558:ASN:HB3	1:A:561:SER:HB3	1.91	0.52
1:A:777:TYR:O	1:A:781:VAL:HG23	2.09	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:170:ILE:C	1:A:171:ARG:HD2	2.31	0.52
1:A:235:ASN:CG	1:A:237:THR:HG23	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:420:LYS:N	1:A:420:LYS:HD2	2.25	0.51
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:160:ARG:HB2	1:A:243:LEU:HB3	1.91	0.51
1:B:133:ASN:ND2	1:B:569:ARG:NH2	2.41	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:521:LEU:HB3	1:A:802:LEU:HD11	1.92	0.51
1:A:527:ASP:O	1:A:531:LEU:HD23	2.11	0.51
1:A:24:VAL:O	1:A:28:LYS:HG3	2.11	0.51
1:A:419:PRO:HB2	1:A:420:LYS:HD2	1.93	0.50
1:A:543:LEU:O	1:A:547:GLN:HG3	2.11	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:380:LEU:HD22	1:A:380:LEU:H	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:OD1	1:A:119:ILE:HD13	2.12	0.50
1:A:433:GLU:HB3	1:A:437:LYS:HD2	1.93	0.50
1:A:789:GLN:HE21	1:A:789:GLN:CA	2.04	0.50
1:B:380:LEU:HD22	1:B:380:LEU:N	2.27	0.50
1:A:296:GLU:OE2	1:A:385:GLU:OE1	2.29	0.49
1:B:678:ASN:HD22	1:B:678:ASN:N	2.09	0.49
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.49
1:A:661:ASP:O	1:A:797:TRP:HH2	1.95	0.49
1:A:678:ASN:ND2	1:A:679:MET:HG3	2.27	0.49
1:A:763:ASN:HB2	6:A:2649:HOH:O	2.11	0.49
1:B:284:ASN:ND2	6:B:2008:HOH:O	2.44	0.49
1:A:431:ILE:N	1:A:431:ILE:HD12	2.27	0.49
1:B:433:GLU:HB3	1:B:437:LYS:HD2	1.94	0.49
1:B:543:LEU:O	1:B:547:GLN:HG3	2.13	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:B:687:LEU:HD12	1:B:797:TRP:CE2	2.48	0.49
1:A:133:ASN:ND2	1:A:281:PRO:HA	2.13	0.49
1:B:346:ILE:HD13	1:B:448:GLY:HA3	1.94	0.49
1:B:488:PRO:O	1:B:492:LEU:HB3	2.12	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:HG23	1:A:65:GLY:H	1.76	0.49
1:A:64:VAL:HG21	1:B:37:PHE:CD1	2.47	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:A:605:ILE:HG21	1:A:623:ILE:HD13	1.93	0.49
1:B:304:LEU:HD12	1:B:348:GLU:HG3	1.95	0.49
1:B:399:HIS:HD2	6:B:2009:HOH:O	1.96	0.49
1:B:275:ILE:O	1:B:295:GLN:HG2	2.13	0.48
1:B:431:ILE:N	1:B:431:ILE:HD12	2.28	0.48
1:A:67:TRP:HA	1:A:238:VAL:HB	1.96	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: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:483:THR:O	1:B:815:ARG:NH2	2.41	0.48
1:B:630:VAL:O	1:B:636:VAL:HG21	2.13	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:A:91:MET:HB2	1:A:129:ALA:HB3	1.95	0.48
1:A:380:LEU:HD22	1:A:380:LEU:N	2.29	0.48
1:A:767:TYR:HB2	1:A:768:HIS:CE1	2.49	0.48
1:B:286:PHE:CE1	1:B:385:GLU:HG3	2.49	0.48
1:A:286:PHE:CE1	1:A:385:GLU:HG3	2.49	0.47
1:B:455:VAL:HG23	1:B:674:SER:HB2	1.95	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:64:VAL:HG23	1:B:65:GLY:H	1.78	0.47
1:B:235:ASN:O	1:B:236:ASN:HB2	2.13	0.47
1:B:661:ASP:O	1:B:797:TRP:HH2	1.96	0.47
1:B:678:ASN:ND2	1:B:679:MET:HG3	2.29	0.47
1:A:389:VAL:HG11	1:A:404:TYR:OH	2.15	0.47
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.79	0.47
1:B:216:ILE:HB	6:B:2373:HOH:O	2.15	0.47
1:B:626:VAL:O	1:B:630:VAL:HG13	2.14	0.47
1:A:136:LEU:HD23	1:A:136:LEU:C	2.35	0.47
1:A:754:GLN:NE2	1:A:757:LEU:HD13	2.30	0.47
1:A:174:TRP:CD2	1:A:621:LYS:HG3	2.50	0.47
1:A:605:ILE:O	1:A:644:PHE:HA	2.14	0.47
1:B:66:ARG:HD2	1:B:236:ASN:HA	1.97	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:72:GLN:HE21	1:A:76:ASP:CG	2.18	0.47
1:A:561:SER:HB2	1:A:601:ARG:HA	1.96	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:455:VAL:H	1:B:459:HIS:CD2	2.31	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:507:ILE:HG13	6:B:2377:HOH:O	2.14	0.46
1:B:697:VAL:O	1:B:701:GLU:HG3	2.15	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:B:561:SER:HB2	1:B:601:ARG:HA	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: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:791:TYR:HA	1:B:797:TRP:CD1	2.51	0.46
1:B:566:GLN:NE2	1:B:576:GLN:HA	2.28	0.45
1:B:579:ASN:C	1:B:579:ASN:HD22	2.19	0.45
1:B:764:MET:CE	1:B:765:LEU:HD13	2.46	0.45
1:A:424:ARG:HD2	1:A:428:MET:SD	2.56	0.45
1:B:422:VAL:HG23	1:B:423:ASP:N	2.31	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:B:630:VAL:HG23	1:B:631:ASN:N	2.30	0.45
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.99	0.45
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.16	0.45
1:A:492:LEU:HD13	1:A:500:ALA:HB2	1.98	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:296:GLU:OE2	1:B:385:GLU:OE1	2.35	0.45
1:B:569:ARG:O	1:B:574:LYS:HD2	2.16	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:A:235:ASN:ND2	1:A:237:THR:H	2.15	0.45
1:A:435:GLY:O	1:A:436:SER:CB	2.64	0.45
1:A:793:ASN:C	1:A:793:ASN:ND2	2.70	0.45
1:B:174:TRP:CD2	1:B:621:LYS:HG3	2.52	0.45
1:B:210:ASN:N	1:B:210:ASN:ND2	2.52	0.45
1:B:402:ILE:O	1:B:406:ILE:HG13	2.17	0.45
1:B:827:VAL:CG1	1:B:828:GLU:N	2.79	0.45
1:A:133:ASN:HD21	1:A:281:PRO:CA	2.16	0.44
1:A:422:VAL:HG23	1:A:423:ASP:N	2.31	0.44
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.99	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:A:196:PHE:HD1	1:A:309:ARG:HH11	1.66	0.44
1:A:636:VAL:HG23	1:A:637:GLY:N	2.32	0.44
1:B:330:PRO:HB3	1:B:370:LYS:HB3	1.99	0.44
1:B:396:LEU:HB3	1:B:399:HIS:CD2	2.53	0.44
1:B:678:ASN:ND2	1:B:678:ASN:N	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:336:GLN:OE1	1:B:373:ALA:HB3	2.17	0.44
1:B:690:GLY:O	1:B:710:ILE:HA	2.18	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:C	1:B:136:LEU:HD23	2.38	0.44
1:A:325:VAL:HG23	1:A:326:PHE:CD1	2.52	0.44
1:A:678:ASN:ND2	1:A:678:ASN:N	2.66	0.44
1:A:713:MET:HB3	1:A:717:ASP:HB2	2.00	0.44
1:B:43:ARG:NH2	1:B:115:LEU:HB3	2.32	0.44
1:B:569:ARG:HD2	1:B:608:LYS:O	2.17	0.44
1:A:112:ILE:HG23	1:A:117:LEU:HB2	1.99	0.44
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.83	0.43
1:A:274:ASN:ND2	1:A:277:ARG:HE	2.15	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:A:735:LEU:HA	1:A:736:PRO:HD2	1.87	0.43
1:B:143:PHE:O	1:B:147:MET:HG3	2.18	0.43
1:B:435:GLY:O	1:B:436:SER:CB	2.66	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:492:LEU:HD13	1:B:500:ALA:HB2	1.99	0.43
1:B:565:VAL:HG11	1:B:660:THR:HG22	1.99	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:492:LEU:HD12	1:B:493:LEU:HD23	2.00	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:29:LYS:HE2	1:B:33:ARG:HH12	1.77	0.43
1:B:83:TYR:HE1	1:B:310:ARG:HH21	1.64	0.43
1:B:746:ASP:OD2	1:B:762:ILE:HG21	2.18	0.43
1:A:36:HIS:HD2	6:A:2604:HOH:O	2.00	0.43
1:A:74:TYR:CZ	1:A:153:ALA:HA	2.53	0.43
1:A:579:ASN:C	1:A:579:ASN:HD22	2.20	0.43
1:B:235:ASN:ND2	1:B:237:THR:HG23	2.34	0.43
1:B:662:LEU:CD2	1:B:689:ILE:HG22	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ILE:HD13	1:A:448:GLY:HA3	2.00	0.43
1:A:510:ASP:HB2	6:A:2379:HOH:O	2.19	0.43
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: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:A:386:ARG:HA	1:A:439:ILE:O	2.19	0.42
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: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:B:793:ASN:C	1:B:793:ASN:ND2	2.72	0.42
1:A:492:LEU:HD12	1:A:493:LEU:HD23	2.01	0.42
1:A:569:ARG:HD2	1:A:608:LYS:O	2.19	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:43:ARG:HD2	1:B:51:TYR:OH	2.20	0.42
1:B:626:VAL:O	1:B:629:VAL:HG13	2.19	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:A:764:MET:C	1:A:764:MET:SD	2.99	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:690:GLY:O	1:A:710:ILE:HA	2.19	0.42
1:B:133:ASN:HD21	1:B:281:PRO:CA	2.16	0.42
1:B:300:VAL:HG13	1:B:345:ALA:HA	2.02	0.41
1:B:415:VAL:HG23	1:B:416:ALA:N	2.35	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:225:PRO:HD3	1:B:244:TRP:CZ3	2.55	0.41
1:B:720:ALA:O	1:B:723:LYS:HB3	2.21	0.41
1:A:754:GLN:N	1:A:755:PRO:HD3	2.35	0.41
1:A:206:VAL:HG23	1:A:397:PRO:HB2	2.02	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:A:378:THR:HA	6:A:2334:HOH:O	2.19	0.41
1:A:517:GLN:OE1	1:A:520:LYS:HE3	2.21	0.41
1:B:304:LEU:O	1:B:308:ILE:HG12	2.20	0.41
1:B:574:LYS:NZ	1:B:672:GLU:OE2	2.53	0.41
1:B:712:GLY:HA2	6:B:2606:HOH:O	2.20	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:339:ASP:O	1:B:342:PRO:HD2	2.21	0.41
1:B:395:LEU:O	1:B:396:LEU:HD13	2.21	0.41
1:B:396:LEU:HD22	1:B:396:LEU:N	2.36	0.41
1:A:395:LEU:O	1:A:396:LEU:HD13	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:B:325:VAL:HG23	1:B:326:PHE:CD1	2.56	0.41
1:B:386:ARG:HA	1:B:439:ILE:O	2.20	0.41
1:B:542:LYS:NZ	6:B:2703:HOH:O	2.53	0.41
1:A:36:HIS:O	1:A:40:VAL:HA	2.21	0.41
1:A:407:ASN:ND2	1:A:431:ILE:HD13	2.36	0.41
1:A:630:VAL:CG2	1:A:631:ASN:N	2.83	0.41
1:B:42:ASP:HB2	6:B:2717:HOH:O	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:785:ASP:O	1:B:789:GLN:HG2	2.20	0.41
1:A:66:ARG:HD2	1:A:236:ASN:HA	2.00	0.41
1:A:355:ASP:HA	6:A:2399:HOH:O	2.19	0.41
1:A:626:VAL:O	1:A:629:VAL:HG13	2.21	0.41
1:B:100:ILE:HD12	1:B:494:LEU:CD2	2.50	0.41
1:B:410:HIS:O	1:B:414:ILE:HD13	2.21	0.41
1:B:615:MET:O	1:B:619:ILE:HG13	2.21	0.41
1:A:423:ASP:OD2	1:A:426:ARG:NE	2.47	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:B:662:LEU:C	1:B:662:LEU:CD2	2.87	0.40
1:A:574:LYS:NZ	1:A:672:GLU:OE2	2.53	0.40
1:B:36:HIS:O	1:B:40:VAL:HA	2.22	0.40
1:B:415:VAL:CG1	1:B:425:LEU:HD11	2.48	0.40
1:A:109:ASP:CB	6:A:2581:HOH:O	2.57	0.40
1:A:161:TYR:HA	1:A:276:SER:O	2.22	0.40
1:B:280:TYR:OH	1:B:291:LEU:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:HG23	1:B:459:HIS:N	2.36	0.40
1:B:687:LEU:HD23	1:B:687:LEU:HA	1.92	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%)	30	34
1	B	779/847 (92%)	733 (94%)	44 (6%)	2 (0%)	37	42
All	All	1558/1694 (92%)	1470 (94%)	83 (5%)	5 (0%)	37	42

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%)	16	19
1	B	688/740 (93%)	645 (94%)	43 (6%)	15	17
All	All	1376/1480 (93%)	1292 (94%)	84 (6%)	15	18

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

Sometimes 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 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	MPD	B	1902	-	7,7,7	0.74	0	9,10,10	0.71	0
3	CP4	A	862	-	33,37,37	1.87	10 (30%)	40,50,50	1.92	10 (25%)
4	PLP	B	1860	1	15,15,16	1.99	2 (13%)	21,22,23	1.39	2 (9%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.08	1 (4%)
2	NBG	B	1861	-	15,15,15	1.54	3 (20%)	21,21,21	1.23	2 (9%)
4	PLP	A	860	1	15,15,16	1.61	2 (13%)	21,22,23	1.28	3 (14%)

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	MPD	B	1902	-	1/1/2/2	2/5/5/5	-
3	CP4	A	862	-	-	2/15/21/21	0/4/4/4
4	PLP	B	1860	1	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/6/26/26	0/1/1/1
2	NBG	B	1861	-	-	0/6/26/26	0/1/1/1
4	PLP	A	860	1	-	1/6/6/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1860	PLP	C4A-C4	-6.16	1.39	1.51
4	A	860	PLP	C4A-C4	-4.41	1.42	1.51
2	A	861	NBG	C2-C1	4.01	1.57	1.53
3	A	862	CP4	C30-C32	3.74	1.43	1.36
3	A	862	CP4	C3-C7	3.70	1.43	1.36
3	A	862	CP4	C5-C8	3.46	1.44	1.36
3	A	862	CP4	C31-C32	3.27	1.44	1.38
3	A	862	CP4	C29-C31	3.23	1.43	1.36
2	B	1861	NBG	C1-N1	3.21	1.47	1.43
2	B	1861	NBG	C2-C1	3.15	1.56	1.53
3	A	862	CP4	C8-C7	3.06	1.43	1.38
3	A	862	CP4	C2-C6	-2.84	1.34	1.39
3	A	862	CP4	C2-C0	2.69	1.51	1.41
3	A	862	CP4	C26-C28	2.67	1.51	1.41
2	A	861	NBG	C3-C2	2.31	1.58	1.52
4	B	1860	PLP	C5A-C5	2.26	1.56	1.50
2	A	861	NBG	C1-N1	2.19	1.46	1.43
2	B	1861	NBG	C3-C2	2.14	1.57	1.52
3	A	862	CP4	C26-C23	-2.12	1.36	1.39
4	A	860	PLP	P-O3P	-2.04	1.47	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	862	CP4	C23-C22-N21	4.48	121.79	115.56
3	A	862	CP4	C2-C0-C1	-4.19	102.62	106.27
3	A	862	CP4	C6-C9-N11	3.96	121.07	115.56
3	A	862	CP4	C26-C28-C27	-3.90	102.87	106.27
3	A	862	CP4	C6-N4-C1	3.72	112.20	104.45
2	A	861	NBG	C5-O5-C1	3.63	117.52	112.47
3	A	862	CP4	C23-N25-C27	3.58	111.92	104.45
2	B	1861	NBG	C5-O5-C1	3.53	117.38	112.47
3	A	862	CP4	C31-C29-C27	-3.05	117.15	120.80
4	B	1860	PLP	O4P-C5A-C5	-3.00	103.74	109.36
3	A	862	CP4	C8-C5-C1	-2.99	117.22	120.80
4	A	860	PLP	O2P-P-O4P	-2.48	100.19	106.67
4	A	860	PLP	O3P-P-O2P	2.39	116.75	107.80
4	A	860	PLP	O4P-C5A-C5	-2.31	105.02	109.36
2	B	1861	NBG	C3-C2-C1	2.24	113.15	109.86
3	A	862	CP4	O24-C22-C23	-2.21	116.20	121.08
4	B	1860	PLP	O3P-P-O4P	-2.12	101.14	106.67
3	A	862	CP4	O12-C9-C6	-2.11	116.42	121.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1902	MPD	C4

All (5) torsion outliers are listed below:

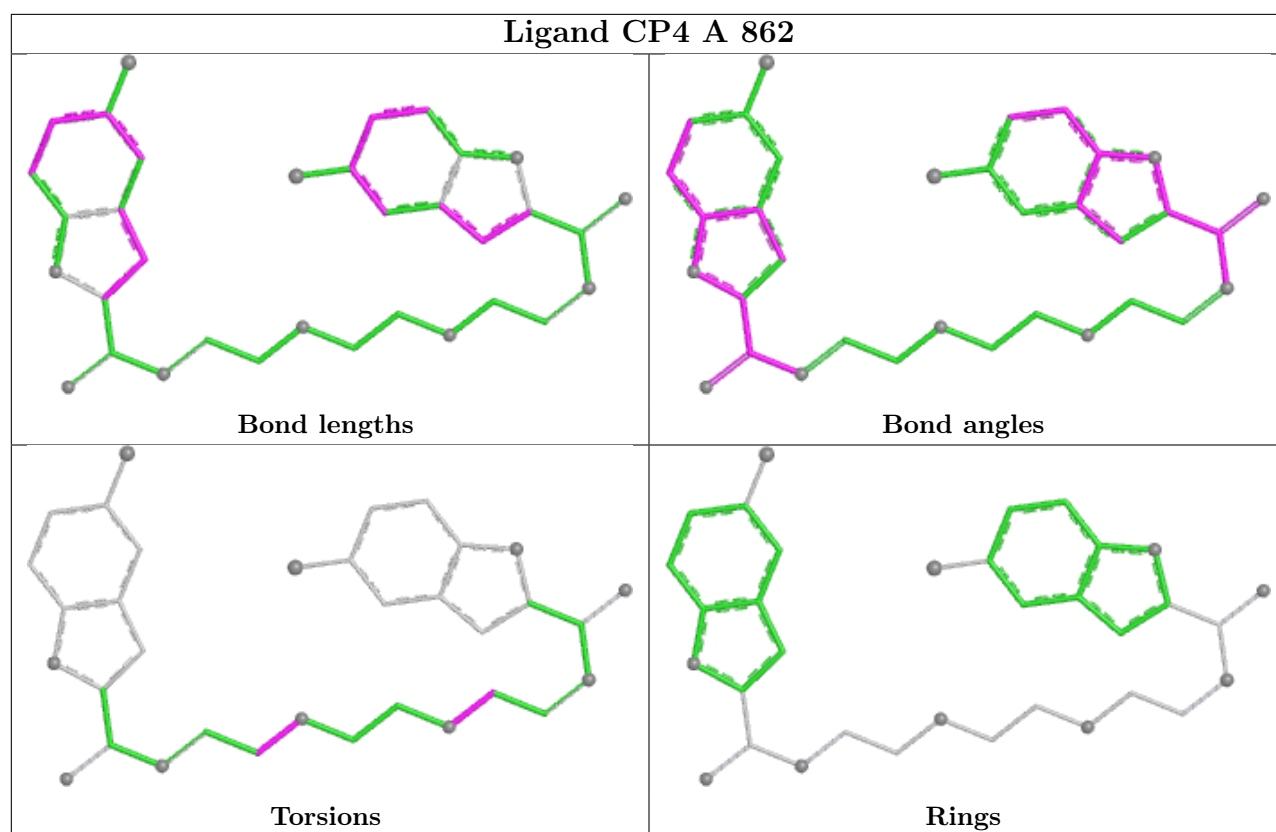
Mol	Chain	Res	Type	Atoms
5	B	1902	MPD	C2-C3-C4-O4
5	B	1902	MPD	C2-C3-C4-C5
4	A	860	PLP	C4-C5-C5A-O4P
3	A	862	CP4	C20-C19-O18-C17
3	A	862	CP4	C13-C14-O15-C16

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.