



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:47 PM UTC

PDB ID : 7TA1 / pdb_00007ta1
Title : Human Ornithine Aminotransferase (hOAT) soaked with gamma-Aminobutyric acid
Authors : Butrin, A.; Wawrzak, Z.; Liu, D.
Deposited on : 2021-12-20
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

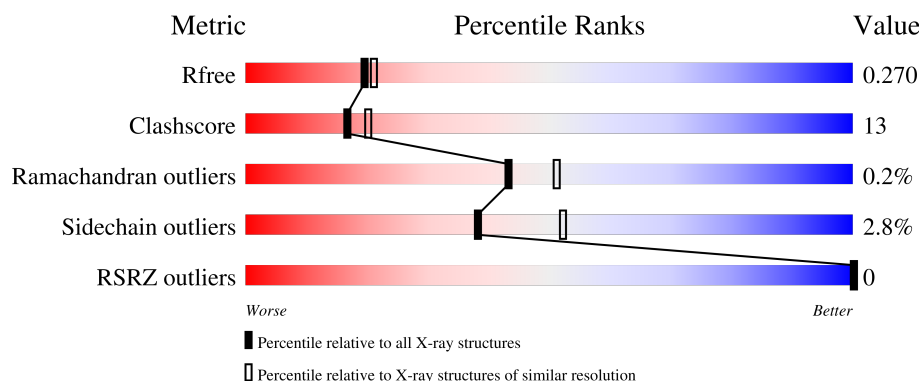
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	439	 71% 19% • 8%
1	B	439	 71% 19% • 8%
1	C	439	 71% 21% 8%
1	D	439	 73% 17% • 8%
1	E	439	 66% 25% • 8%

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Mol	Chain	Length	Quality of chain
1	F	439	65% 26% • 8%

2 Entry composition [i](#)

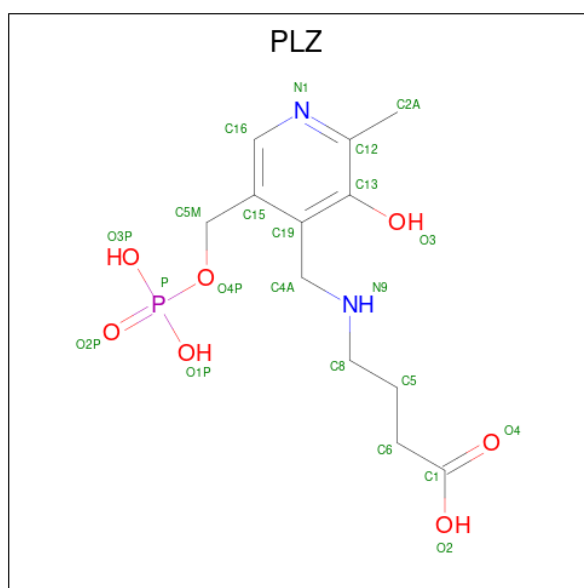
There are 4 unique types of molecules in this entry. The entry contains 19965 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine aminotransferase, mitochondrial.

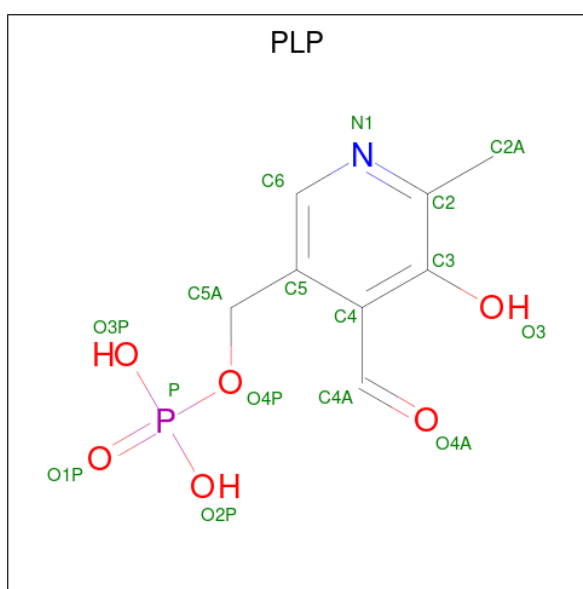
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3161	2030	533	586	12			
1	B	404	Total	C	N	O	S	0	0	0
			3161	2030	533	586	12			
1	C	404	Total	C	N	O	S	0	0	0
			3161	2030	533	586	12			
1	D	402	Total	C	N	O	S	0	0	0
			3150	2023	531	584	12			
1	E	404	Total	C	N	O	S	0	0	0
			3161	2030	533	586	12			
1	F	403	Total	C	N	O	S	0	0	0
			3157	2028	532	585	12			

- Molecule 2 is 4-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL)METHYL)AMINO]BUTANOIC ACID (CCD ID: PLZ) (formula: C₁₂H₁₉N₂O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		
4	B	191	Total	O	0	0
			191	191		
4	C	140	Total	O	0	0
			140	140		

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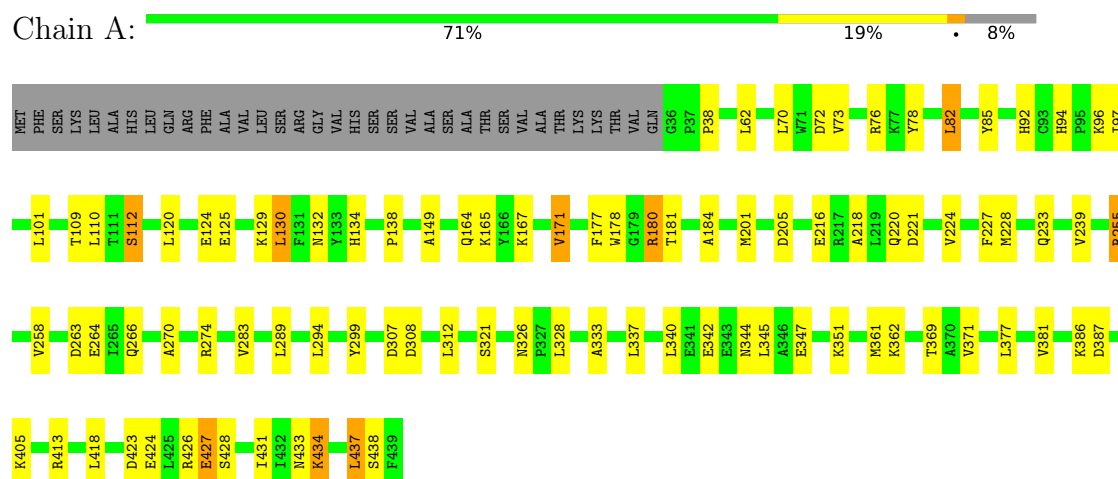
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	137	Total 137	O 137	0	0
4	E	157	Total 157	O 157	0	0
4	F	140	Total 140	O 140	0	0

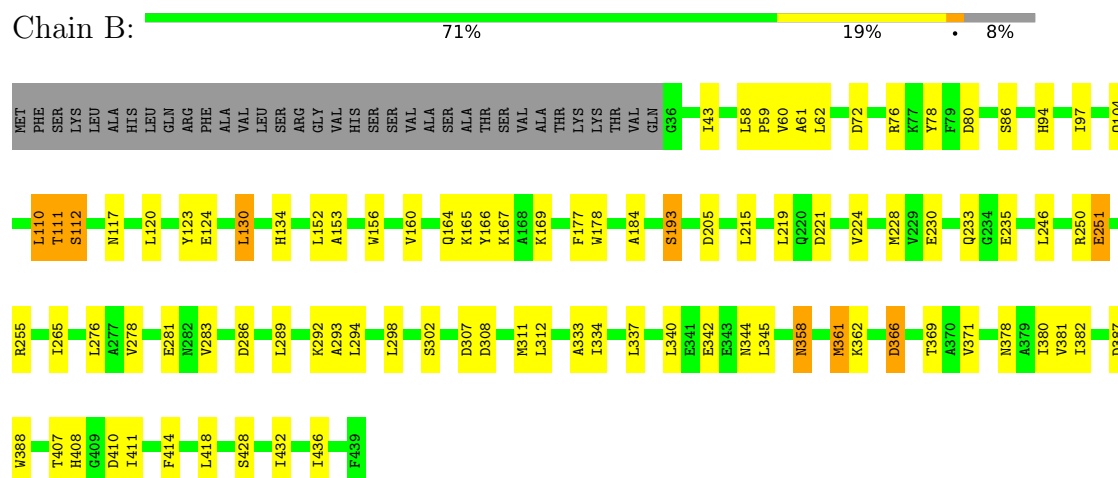
3 Residue-property plots

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

- Molecule 1: Ornithine aminotransferase, mitochondrial

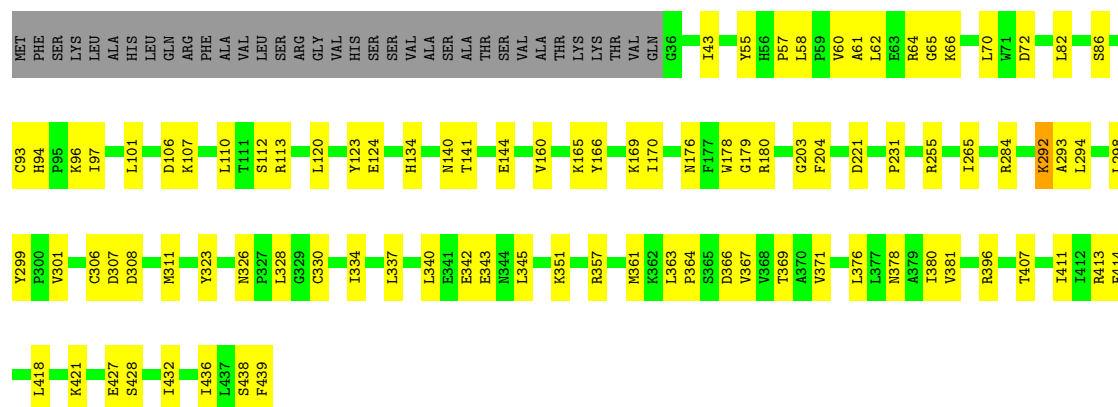


- Molecule 1: Ornithine aminotransferase, mitochondrial



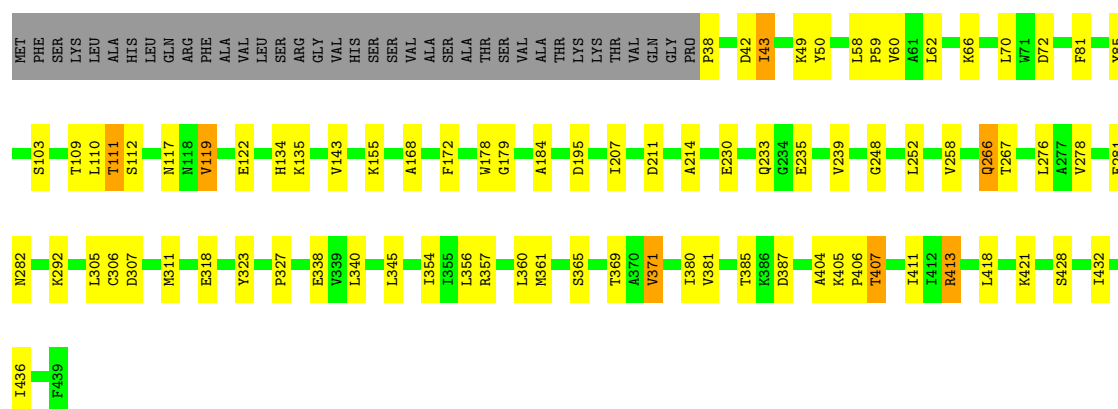
- Molecule 1: Ornithine aminotransferase, mitochondrial





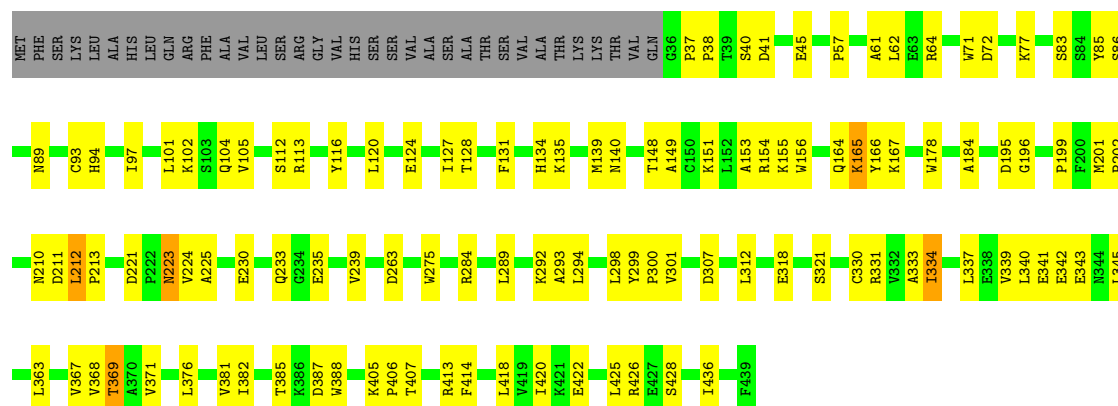
- Molecule 1: Ornithine aminotransferase, mitochondrial

Chain D: 73% 17% 8%



- Molecule 1: Ornithine aminotransferase, mitochondrial

Chain E: 66% 25% 8%



- Molecule 1: Ornithine aminotransferase, mitochondrial

Chain F: 65% 26% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.61Å 114.61Å 349.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.25 – 2.20 99.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (99.25-2.20) 99.8 (99.25-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.02Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.251 , 0.268 0.251 , 0.270	Depositor DCC
R_{free} test set	8827 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.119 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19965	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLZ, 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	0.21	0/3235	0.47	0/4393
1	B	0.24	1/3235 (0.0%)	0.44	0/4393
1	C	0.18	0/3235	0.43	0/4393
1	D	0.18	0/3223	0.41	0/4375
1	E	0.22	1/3235 (0.0%)	0.45	0/4393
1	F	0.22	0/3231	0.43	0/4387
All	All	0.21	2/19394 (0.0%)	0.44	0/26334

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	ASP	CB-CG	-6.91	1.34	1.52
1	E	212	LEU	C-N	5.20	1.41	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3161	0	3165	77	1
1	B	3161	0	3165	77	0
1	C	3161	0	3163	88	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3150	0	3156	67	1
1	E	3161	0	3165	93	0
1	F	3157	0	3163	104	1
2	A	22	0	16	3	0
2	B	22	0	16	1	0
2	C	22	0	16	3	0
2	D	22	0	16	2	0
3	E	15	0	7	1	0
3	F	15	0	7	1	0
4	A	131	0	0	28	4
4	B	191	0	0	41	5
4	C	140	0	0	47	1
4	D	137	0	0	35	4
4	E	157	0	0	30	1
4	F	140	0	0	30	1
All	All	19965	0	19055	489	13

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (489) 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:E:307:ASP:OD2	4:E:601:HOH:O	1.84	0.94
1:C:294:LEU:O	4:C:601:HOH:O	1.86	0.94
1:D:42:ASP:OD2	4:D:601:HOH:O	1.89	0.91
1:B:308:ASP:O	4:B:601:HOH:O	1.88	0.90
1:B:294:LEU:HD12	1:B:337:LEU:HD21	1.51	0.90
1:E:196:GLY:O	4:E:602:HOH:O	1.89	0.89
1:A:228:MET:SD	4:A:718:HOH:O	2.30	0.89
1:C:180:ARG:NH1	4:C:612:HOH:O	2.06	0.88
1:C:307:ASP:O	4:C:602:HOH:O	1.93	0.86
1:F:127:ILE:O	4:F:601:HOH:O	1.92	0.86
1:C:221:ASP:O	4:C:603:HOH:O	1.95	0.84
1:D:122:GLU:OE2	4:D:603:HOH:O	1.95	0.83
1:F:165:LYS:NZ	4:F:606:HOH:O	2.10	0.83
1:A:110:LEU:O	4:A:601:HOH:O	1.95	0.83
1:E:164:GLN:HB3	1:E:167:LYS:HE2	1.61	0.82
1:A:294:LEU:HD12	1:A:337:LEU:HD21	1.59	0.82
1:C:306:CYS:SG	4:C:602:HOH:O	2.37	0.82
1:E:41:ASP:OD1	4:E:604:HOH:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:O	4:B:603:HOH:O	1.98	0.82
1:C:284:ARG:NE	4:C:615:HOH:O	2.13	0.81
1:E:127:ILE:O	4:E:603:HOH:O	1.97	0.81
1:C:64:ARG:NH1	1:C:65:GLY:O	2.14	0.80
1:A:387:ASP:OD1	4:A:602:HOH:O	1.99	0.80
1:B:414:PHE:O	4:B:604:HOH:O	1.99	0.80
1:E:318:GLU:O	4:E:606:HOH:O	2.00	0.79
1:A:76:ARG:NH1	1:A:78:TYR:OH	2.14	0.79
1:C:176:ASN:OD1	4:C:606:HOH:O	2.00	0.79
1:C:176:ASN:O	4:C:605:HOH:O	2.00	0.79
4:E:602:HOH:O	1:F:158:TYR:HD2	1.64	0.79
1:F:238:VAL:O	4:F:603:HOH:O	2.01	0.79
1:F:106:ASP:OD2	4:F:602:HOH:O	2.00	0.78
1:B:289:LEU:O	4:B:605:HOH:O	2.01	0.78
1:A:132:ASN:ND2	4:A:608:HOH:O	2.12	0.78
1:C:134:HIS:O	4:C:609:HOH:O	2.02	0.78
1:E:294:LEU:HD12	1:E:337:LEU:HD11	1.66	0.78
1:E:153:ALA:O	4:E:605:HOH:O	2.00	0.77
1:E:230:GLU:OE1	4:E:607:HOH:O	2.01	0.77
1:C:65:GLY:O	4:C:607:HOH:O	2.01	0.77
1:F:234:GLY:O	1:F:413:ARG:NH2	2.17	0.77
1:A:96:LYS:NZ	1:A:342:GLU:OE1	2.17	0.77
1:A:289:LEU:O	4:A:603:HOH:O	2.02	0.77
1:A:274:ARG:N	4:A:612:HOH:O	2.17	0.77
1:C:57:PRO:O	4:C:610:HOH:O	2.03	0.76
1:A:216:GLU:OE2	1:A:220:GLN:NE2	2.18	0.76
1:D:66:LYS:NZ	4:D:614:HOH:O	2.16	0.76
1:B:302:SER:O	4:B:606:HOH:O	2.03	0.76
1:B:312:LEU:N	4:B:601:HOH:O	2.03	0.76
1:A:130:LEU:O	4:A:605:HOH:O	2.04	0.76
1:D:292:LYS:HG3	4:D:615:HOH:O	1.85	0.75
1:C:204:PHE:HA	4:C:614:HOH:O	1.86	0.75
1:C:160:VAL:O	4:C:608:HOH:O	2.02	0.75
1:E:413:ARG:O	4:E:608:HOH:O	2.05	0.74
1:D:306:CYS:O	4:D:605:HOH:O	2.04	0.74
1:C:64:ARG:NH1	4:C:620:HOH:O	2.20	0.74
1:B:265:ILE:HG13	4:B:605:HOH:O	1.86	0.74
1:F:435:THR:O	4:F:605:HOH:O	2.05	0.74
1:C:96:LYS:NZ	1:C:342:GLU:OE1	2.21	0.74
1:F:344:ASN:ND2	4:F:613:HOH:O	2.20	0.74
1:E:94:HIS:HB3	1:E:97:ILE:HD13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:PRO:O	4:F:604:HOH:O	2.04	0.73
1:B:278:VAL:HB	1:B:283:VAL:HG13	1.70	0.73
1:E:148:THR:OG1	4:E:609:HOH:O	2.06	0.73
1:C:97:ILE:HG22	1:C:298:LEU:HD12	1.69	0.73
1:B:358:ASN:OD1	4:B:607:HOH:O	2.05	0.73
1:F:113:ARG:NH1	4:F:612:HOH:O	2.20	0.73
1:C:371:VAL:HG22	1:C:380:ILE:HG22	1.71	0.72
1:B:265:ILE:N	4:B:605:HOH:O	2.21	0.72
1:A:181:THR:OG1	4:A:604:HOH:O	2.03	0.72
1:A:205:ASP:OD2	4:A:606:HOH:O	2.06	0.72
1:C:101:LEU:HD12	1:C:328:LEU:HD11	1.69	0.71
1:D:38:PRO:HA	4:D:601:HOH:O	1.90	0.71
1:D:109:THR:O	4:D:602:HOH:O	2.07	0.71
1:E:116:TYR:CE1	1:F:57:PRO:HG2	2.25	0.71
1:F:228:MET:HG3	1:F:261:ILE:HB	1.70	0.71
1:E:195:ASP:OD1	4:E:610:HOH:O	2.07	0.71
1:F:349:ALA:HA	1:F:376:LEU:HD23	1.72	0.71
1:C:93:CYS:HB2	4:C:607:HOH:O	1.90	0.71
1:C:169:LYS:NZ	4:C:626:HOH:O	2.24	0.71
1:E:57:PRO:HG2	1:F:116:TYR:CE1	2.26	0.71
1:D:172:PHE:O	4:D:606:HOH:O	2.09	0.70
1:A:177:PHE:HE1	2:A:501:PLZ:H4A2	1.55	0.70
1:C:203:GLY:O	4:C:614:HOH:O	2.09	0.70
1:E:275:TRP:HZ2	1:E:341:GLU:HG2	1.56	0.70
1:D:207:ILE:HD12	4:D:620:HOH:O	1.90	0.70
1:B:286:ASP:OD1	4:B:609:HOH:O	2.09	0.70
1:F:228:MET:HG3	1:F:261:ILE:CG2	2.22	0.70
1:B:228:MET:O	4:B:610:HOH:O	2.09	0.69
1:C:414:PHE:O	4:C:613:HOH:O	2.08	0.69
1:E:40:SER:O	4:E:611:HOH:O	2.10	0.69
1:E:405:LYS:HD2	1:E:406:PRO:HD2	1.73	0.69
1:D:111:THR:HG21	1:D:117:ASN:HB3	1.75	0.69
1:A:180:ARG:NH2	4:A:617:HOH:O	2.25	0.69
1:D:405:LYS:HD2	1:D:406:PRO:HD2	1.75	0.69
1:B:97:ILE:HG22	1:B:298:LEU:HD12	1.73	0.68
1:B:255:ARG:NE	4:B:629:HOH:O	2.26	0.68
1:A:437:LEU:HD13	4:A:619:HOH:O	1.93	0.68
1:B:342:GLU:OE2	4:B:612:HOH:O	2.11	0.68
1:A:62:LEU:HA	1:A:72:ASP:HA	1.76	0.68
2:C:501:PLZ:HN9	2:C:501:PLZ:H5M1	1.59	0.68
1:B:251:GLU:OE2	1:B:255:ARG:NH2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:THR:O	4:B:613:HOH:O	2.11	0.67
1:D:340:LEU:O	4:D:608:HOH:O	2.12	0.67
1:D:385:THR:OG1	1:D:387:ASP:OD1	2.11	0.67
1:D:258:VAL:O	4:D:609:HOH:O	2.12	0.67
1:E:420:ILE:O	4:E:612:HOH:O	2.12	0.67
1:E:101:LEU:HD21	1:F:101:LEU:HD21	1.75	0.66
1:F:377:LEU:HD11	1:F:413:ARG:HH11	1.59	0.66
1:C:106:ASP:OD2	4:C:616:HOH:O	2.14	0.66
1:E:414:PHE:O	4:E:613:HOH:O	2.13	0.66
1:F:371:VAL:HG22	1:F:380:ILE:HG22	1.77	0.66
1:A:201:MET:O	4:A:609:HOH:O	2.14	0.65
1:B:366:ASP:OD1	4:B:614:HOH:O	2.14	0.65
1:D:405:LYS:O	4:D:611:HOH:O	2.13	0.65
1:B:111:THR:HG21	1:B:117:ASN:HB3	1.77	0.65
1:E:165:LYS:NZ	1:F:195:ASP:OD1	2.27	0.65
1:D:168:ALA:O	4:D:612:HOH:O	2.13	0.65
1:D:81:PHE:O	4:D:610:HOH:O	2.12	0.65
1:F:69:TYR:OH	4:F:607:HOH:O	2.12	0.65
1:A:112:SER:O	4:A:610:HOH:O	2.14	0.65
1:F:236:ALA:HB2	4:F:631:HOH:O	1.97	0.65
1:F:385:THR:OG1	1:F:387:ASP:OD1	2.13	0.65
1:A:177:PHE:CE1	2:A:501:PLZ:H4A2	2.32	0.64
1:B:235:GLU:OE1	4:B:615:HOH:O	2.15	0.64
1:B:281:GLU:OE2	4:B:616:HOH:O	2.15	0.64
4:E:602:HOH:O	1:F:155:LYS:HA	1.97	0.64
1:F:140:ASN:OD1	4:F:608:HOH:O	2.15	0.64
1:F:377:LEU:HD11	1:F:413:ARG:NH1	2.12	0.64
1:A:125:GLU:HG3	1:A:129:LYS:HE3	1.79	0.64
1:A:218:ALA:O	4:A:611:HOH:O	2.14	0.63
1:F:228:MET:HG3	1:F:261:ILE:CB	2.27	0.63
1:C:66:LYS:HA	4:C:607:HOH:O	1.98	0.63
1:B:235:GLU:O	4:B:617:HOH:O	2.15	0.63
1:B:215:LEU:HD11	4:B:719:HOH:O	1.98	0.62
1:E:128:THR:O	4:E:614:HOH:O	2.16	0.62
1:B:76:ARG:NH2	4:B:643:HOH:O	2.32	0.62
1:A:134:HIS:HB2	1:A:307:ASP:HA	1.81	0.62
1:A:101:LEU:HD12	1:A:328:LEU:HD11	1.81	0.61
1:E:385:THR:OG1	1:E:387:ASP:OD1	2.18	0.61
1:B:289:LEU:C	4:B:605:HOH:O	2.40	0.61
1:E:97:ILE:HD11	1:E:339:VAL:HG21	1.82	0.61
1:E:61:ALA:HB2	4:E:611:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:LEU:O	4:D:613:HOH:O	2.16	0.61
1:C:66:LYS:NZ	4:C:630:HOH:O	2.27	0.61
1:F:284:ARG:NH1	4:F:604:HOH:O	2.34	0.61
1:C:94:HIS:HB3	1:C:97:ILE:HD12	1.82	0.60
1:A:164:GLN:HB3	1:A:167:LYS:HD3	1.84	0.60
1:D:282:ASN:HD22	1:E:284:ARG:NH2	2.00	0.60
1:E:77:LYS:NZ	4:E:634:HOH:O	2.34	0.60
1:B:104:GLN:OE1	4:B:618:HOH:O	2.17	0.60
1:E:38:PRO:O	4:E:615:HOH:O	2.16	0.60
1:E:275:TRP:CZ2	1:E:341:GLU:HG2	2.36	0.59
1:A:109:THR:OG1	4:A:607:HOH:O	2.11	0.59
1:E:210:ASN:ND2	4:E:636:HOH:O	2.34	0.59
1:C:255:ARG:NH2	4:C:636:HOH:O	2.36	0.59
1:F:348:ASN:HA	4:F:644:HOH:O	2.03	0.59
1:D:360:LEU:HD12	4:D:703:HOH:O	2.02	0.59
1:E:101:LEU:CD2	1:F:101:LEU:HD21	2.32	0.59
1:C:255:ARG:NH1	4:C:629:HOH:O	2.26	0.58
1:F:234:GLY:C	1:F:413:ARG:HH22	2.10	0.58
1:F:101:LEU:O	1:F:105:VAL:HG23	2.03	0.58
1:A:270:ALA:HA	4:A:612:HOH:O	2.01	0.58
1:A:347:GLU:O	1:A:351:LYS:HG2	2.04	0.58
1:C:311:MET:N	4:C:602:HOH:O	2.34	0.58
1:E:300:PRO:HD3	1:F:299:TYR:CZ	2.38	0.58
1:C:140:ASN:HB2	4:C:641:HOH:O	2.04	0.57
1:C:170:ILE:O	4:C:614:HOH:O	2.17	0.57
1:E:134:HIS:HB2	1:E:307:ASP:HA	1.87	0.57
1:E:225:ALA:HB1	4:E:605:HOH:O	2.04	0.57
1:E:363:LEU:HD22	1:E:436:ILE:HG21	1.87	0.57
1:B:80:ASP:N	4:B:620:HOH:O	2.38	0.57
1:B:193:SER:O	4:B:619:HOH:O	2.17	0.57
1:E:211:ASP:OD1	1:E:213:PRO:HD2	2.04	0.57
1:B:134:HIS:HB2	1:B:307:ASP:HA	1.87	0.56
1:B:292:LYS:HB2	4:B:656:HOH:O	2.05	0.56
1:C:378:ASN:HB2	4:C:613:HOH:O	2.05	0.56
1:B:160:VAL:HG11	4:B:626:HOH:O	2.05	0.56
1:C:55:TYR:HH	2:C:501:PLZ:C1	2.18	0.56
1:F:134:HIS:HB2	1:F:307:ASP:HA	1.88	0.56
1:F:247:MET:HG3	1:F:281:GLU:HB3	1.88	0.56
1:A:264:GLU:HB2	4:A:603:HOH:O	2.05	0.56
1:A:274:ARG:NH2	4:A:614:HOH:O	2.23	0.56
1:C:134:HIS:HB2	1:C:307:ASP:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:ARG:O	1:F:361:MET:HG3	2.06	0.56
1:F:149:ALA:HB2	1:F:289:LEU:HD21	1.88	0.56
1:D:135:LYS:HB2	4:D:605:HOH:O	2.06	0.55
1:B:156:TRP:HB3	4:B:603:HOH:O	2.05	0.55
1:C:357:ARG:O	1:C:361:MET:HG3	2.06	0.55
1:D:365:SER:OG	4:D:607:HOH:O	2.11	0.55
1:A:130:LEU:HD23	4:A:605:HOH:O	2.06	0.55
1:B:169:LYS:HE3	1:B:205:ASP:OD2	2.06	0.55
1:C:82:LEU:HD12	1:C:413:ARG:NH1	2.20	0.55
1:C:438:SER:O	1:C:439:PHE:HB2	2.07	0.55
1:A:345:LEU:HD13	1:A:418:LEU:HB2	1.89	0.55
1:C:294:LEU:HB3	4:C:627:HOH:O	2.07	0.55
1:C:231:PRO:O	4:C:617:HOH:O	2.17	0.55
1:F:38:PRO:O	1:F:73:VAL:HG21	2.06	0.55
1:E:156:TRP:HE3	4:E:605:HOH:O	1.90	0.55
1:E:333:ALA:O	1:E:337:LEU:HD13	2.07	0.55
1:A:82:LEU:CD2	1:A:85:TYR:H	2.20	0.54
1:C:396:ARG:NH1	1:C:438:SER:OG	2.40	0.54
1:A:82:LEU:HD23	1:A:85:TYR:H	1.72	0.54
1:A:94:HIS:HB3	1:A:97:ILE:HD12	1.88	0.54
1:E:223:ASN:HD22	1:E:223:ASN:N	2.06	0.54
1:B:130:LEU:HD21	1:B:337:LEU:HD12	1.89	0.54
1:B:246:LEU:HD23	1:B:278:VAL:HG12	1.89	0.54
1:E:300:PRO:HG2	1:F:300:PRO:HG2	1.89	0.54
1:F:131:PHE:N	4:F:601:HOH:O	2.01	0.54
1:F:424:GLU:HG2	4:F:607:HOH:O	2.08	0.54
1:A:333:ALA:O	1:A:337:LEU:HD23	2.08	0.54
1:A:321:SER:O	4:A:613:HOH:O	2.18	0.54
1:E:369:THR:N	1:E:381:VAL:O	2.40	0.54
1:F:340:LEU:HD23	1:F:345:LEU:HD22	1.90	0.54
1:B:156:TRP:HE3	4:B:603:HOH:O	1.90	0.54
1:E:202:PRO:HG2	1:F:199:PRO:HB2	1.90	0.54
1:C:421:LYS:HE2	1:C:421:LYS:HA	1.90	0.53
1:C:178:TRP:HD1	4:C:606:HOH:O	1.90	0.53
1:E:131:PHE:N	4:E:603:HOH:O	2.08	0.53
1:E:151:LYS:NZ	1:F:180:ARG:O	2.41	0.53
1:D:356:LEU:HG	4:D:703:HOH:O	2.08	0.53
1:C:178:TRP:CD1	4:C:606:HOH:O	2.60	0.53
1:F:97:ILE:HD11	1:F:339:VAL:HG21	1.89	0.53
1:C:330:CYS:O	1:C:334:ILE:HD12	2.09	0.53
1:E:89:ASN:N	4:E:630:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:LYS:HE2	1:E:312:LEU:HD21	1.91	0.53
1:D:62:LEU:HA	1:D:72:ASP:HA	1.91	0.53
1:F:284:ARG:HG2	4:F:604:HOH:O	2.09	0.52
1:F:344:ASN:HB3	4:F:613:HOH:O	2.09	0.52
1:F:49:LYS:O	4:F:609:HOH:O	2.19	0.52
1:F:263:ASP:HA	1:F:289:LEU:HB2	1.91	0.52
1:A:178:TRP:CZ2	1:A:184:ALA:HA	2.44	0.52
1:E:340:LEU:HD23	1:E:345:LEU:HD12	1.92	0.52
1:C:113:ARG:NH1	4:C:604:HOH:O	1.99	0.52
1:D:311:MET:HB2	4:D:605:HOH:O	2.10	0.52
1:E:201:MET:HE2	1:F:201:MET:HE2	1.92	0.52
1:B:345:LEU:HD13	1:B:418:LEU:HB2	1.90	0.52
1:A:228:MET:HG2	4:A:703:HOH:O	2.10	0.52
1:C:134:HIS:NE2	4:C:624:HOH:O	2.23	0.52
1:B:371:VAL:HG23	1:B:380:ILE:HG22	1.91	0.51
1:C:204:PHE:HD1	4:C:614:HOH:O	1.93	0.51
1:D:407:THR:OG1	1:D:411:ILE:HB	2.09	0.51
1:F:158:TYR:O	4:F:606:HOH:O	2.19	0.51
1:B:311:MET:N	4:B:601:HOH:O	2.42	0.51
1:E:139:MET:HE1	1:E:321:SER:HB2	1.92	0.51
1:E:330:CYS:O	1:E:334:ILE:HG22	2.11	0.51
1:C:407:THR:OG1	1:C:411:ILE:HB	2.09	0.51
1:F:62:LEU:CD1	1:F:70:LEU:HB3	2.40	0.51
1:A:405:LYS:HZ1	1:A:413:ARG:HH21	1.57	0.51
1:B:62:LEU:HA	1:B:72:ASP:HA	1.93	0.51
1:B:78:TYR:OH	4:B:608:HOH:O	2.06	0.51
1:E:57:PRO:HB3	1:F:113:ARG:O	2.11	0.51
1:E:140:ASN:ND2	4:E:639:HOH:O	2.38	0.51
1:F:52:ALA:O	4:F:611:HOH:O	2.19	0.51
1:F:309:ASP:OD1	4:F:610:HOH:O	2.19	0.51
1:D:345:LEU:HD13	1:D:418:LEU:HB2	1.93	0.51
1:F:407:THR:OG1	1:F:411:ILE:HB	2.11	0.51
1:B:94:HIS:HB3	1:B:97:ILE:HD12	1.93	0.51
1:E:263:ASP:HA	1:E:289:LEU:HB2	1.93	0.51
1:D:267:THR:O	4:D:617:HOH:O	2.19	0.50
1:D:134:HIS:HB2	1:D:307:ASP:HA	1.94	0.50
1:D:404:ALA:HB3	4:D:730:HOH:O	2.10	0.50
2:C:501:PLZ:H5M1	2:C:501:PLZ:N9	2.24	0.50
1:D:338:GLU:OE1	4:D:616:HOH:O	2.19	0.50
1:E:93:CYS:SG	4:E:645:HOH:O	2.48	0.50
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:THR:HG23	4:C:641:HOH:O	2.11	0.50
1:E:37:PRO:C	4:E:615:HOH:O	2.55	0.50
1:B:333:ALA:O	1:B:337:LEU:HD23	2.12	0.50
1:F:69:TYR:CE1	1:F:77:LYS:HE2	2.47	0.50
1:B:382:ILE:HB	1:B:388:TRP:CH2	2.47	0.49
1:F:62:LEU:HD11	1:F:70:LEU:HB3	1.94	0.49
1:B:286:ASP:HA	4:B:714:HOH:O	2.10	0.49
1:C:432:ILE:O	1:C:436:ILE:HG12	2.12	0.49
1:F:238:VAL:HG22	1:F:413:ARG:NH1	2.27	0.49
1:A:263:ASP:HA	1:A:289:LEU:HB2	1.93	0.49
1:C:351:LYS:NZ	4:C:645:HOH:O	2.45	0.49
1:F:391:TRP:HD1	1:F:392:LYS:HE2	1.76	0.49
1:C:337:LEU:HD22	4:C:601:HOH:O	2.12	0.49
1:C:62:LEU:HD13	1:C:70:LEU:HD13	1.94	0.49
1:C:86:SER:OG	4:C:611:HOH:O	2.04	0.49
1:D:62:LEU:HD13	1:D:70:LEU:HD13	1.94	0.49
1:D:155:LYS:NZ	1:D:318:GLU:OE1	2.46	0.49
1:D:211:ASP:HB3	4:D:620:HOH:O	2.12	0.49
1:D:432:ILE:O	1:D:436:ILE:HG12	2.13	0.49
1:E:113:ARG:O	1:F:57:PRO:HB3	2.13	0.49
1:E:345:LEU:HD13	1:E:418:LEU:HB2	1.95	0.49
1:B:78:TYR:O	4:B:620:HOH:O	2.20	0.49
1:B:165:LYS:HA	1:B:166:TYR:HA	1.65	0.49
1:D:62:LEU:HD22	1:D:70:LEU:HB3	1.94	0.49
1:F:178:TRP:CZ2	1:F:184:ALA:HA	2.48	0.49
1:F:240:VAL:HG23	4:F:603:HOH:O	2.12	0.49
1:B:344:ASN:HB3	4:B:680:HOH:O	2.12	0.48
1:C:179:GLY:O	4:C:619:HOH:O	2.20	0.48
1:D:340:LEU:HD23	1:D:345:LEU:HD12	1.95	0.48
1:B:276:LEU:HB3	1:B:278:VAL:HG22	1.94	0.48
1:C:369:THR:N	1:C:381:VAL:O	2.46	0.48
1:D:62:LEU:CD1	1:D:70:LEU:HD13	2.43	0.48
1:F:291:GLY:N	4:F:629:HOH:O	2.37	0.48
1:B:361:MET:HG2	1:B:371:VAL:HG11	1.94	0.48
1:B:407:THR:HG22	1:B:408:HIS:ND1	2.28	0.48
1:E:149:ALA:HB2	1:E:289:LEU:HD21	1.95	0.48
1:D:119:VAL:HG21	1:D:327:PRO:HA	1.94	0.48
1:B:378:ASN:ND2	4:B:604:HOH:O	2.40	0.48
1:F:232:ILE:HG12	1:F:240:VAL:HG22	1.96	0.48
1:E:199:PRO:HB2	1:F:202:PRO:HG2	1.95	0.48
1:D:230:GLU:OE1	1:D:233:GLN:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:LEU:HB2	1:E:368:VAL:HG21	1.96	0.47
1:F:169:LYS:CD	1:F:203:GLY:HA2	2.44	0.47
1:E:263:ASP:OD2	3:E:501:PLP:N1	2.47	0.47
1:E:62:LEU:HA	1:E:72:ASP:HA	1.96	0.47
1:E:97:ILE:HG22	1:E:298:LEU:HD22	1.96	0.47
1:D:207:ILE:N	4:D:606:HOH:O	2.46	0.47
1:D:360:LEU:HB2	4:D:728:HOH:O	2.14	0.47
1:A:426:ARG:O	1:A:427:GLU:HB3	2.15	0.47
1:C:265:ILE:CG2	1:C:292:LYS:HD3	2.45	0.47
1:D:405:LYS:N	4:D:644:HOH:O	2.46	0.47
1:A:433:ASN:O	1:A:434:LYS:HB3	2.15	0.47
1:F:169:LYS:HE3	4:F:704:HOH:O	2.14	0.47
1:F:236:ALA:CB	4:F:631:HOH:O	2.58	0.47
1:D:248:GLY:O	1:D:252:LEU:HD13	2.15	0.47
1:F:165:LYS:H	1:F:165:LYS:HD2	1.80	0.47
1:A:62:LEU:CD1	1:A:70:LEU:HD13	2.46	0.46
1:A:171:VAL:HG13	1:A:227:PHE:HA	1.97	0.46
1:B:164:GLN:HB3	1:B:167:LYS:CE	2.46	0.46
1:B:308:ASP:C	4:B:601:HOH:O	2.50	0.46
1:C:62:LEU:HA	1:C:72:ASP:HA	1.97	0.46
1:D:178:TRP:CZ2	1:D:184:ALA:HA	2.50	0.46
1:D:281:GLU:OE2	4:D:618:HOH:O	2.21	0.46
1:F:376:LEU:HD12	1:F:416:PRO:HD2	1.95	0.46
1:F:94:HIS:HB3	1:F:97:ILE:HD13	1.97	0.46
1:A:38:PRO:O	1:A:73:VAL:HG21	2.15	0.46
1:A:405:LYS:HE2	1:A:405:LYS:HB3	1.79	0.46
1:A:427:GLU:O	1:A:431:ILE:HG13	2.15	0.46
1:E:221:ASP:HB3	1:E:224:VAL:HG23	1.97	0.46
1:B:177:PHE:HB3	4:B:737:HOH:O	2.16	0.46
1:E:85:TYR:O	1:E:292:LYS:HD3	2.15	0.46
1:F:251:GLU:OE2	1:F:255:ARG:NH1	2.48	0.46
1:C:141:THR:N	4:C:641:HOH:O	2.41	0.46
1:C:165:LYS:HA	1:C:166:TYR:HA	1.62	0.46
1:E:382:ILE:HB	1:E:388:TRP:CH2	2.51	0.46
1:D:371:VAL:HG12	1:D:380:ILE:HG22	1.98	0.46
1:E:165:LYS:HA	1:E:166:TYR:HA	1.57	0.46
1:A:377:LEU:HD11	1:A:413:ARG:HH11	1.82	0.45
1:C:340:LEU:HD23	1:C:345:LEU:HD12	1.97	0.45
1:F:85:TYR:O	1:F:292:LYS:HD3	2.15	0.45
1:F:343:GLU:HB2	1:F:345:LEU:CD1	2.46	0.45
1:C:82:LEU:HD12	1:C:413:ARG:HH11	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ILE:HD11	4:D:713:HOH:O	2.16	0.45
1:B:123:TYR:HB2	1:B:334:ILE:HD11	1.97	0.45
1:E:422:GLU:OE2	1:E:426:ARG:NH1	2.48	0.45
1:F:351:LYS:HB2	4:F:644:HOH:O	2.16	0.45
1:B:432:ILE:O	1:B:436:ILE:HG12	2.16	0.45
1:C:170:ILE:HB	4:C:614:HOH:O	2.16	0.45
1:F:165:LYS:HA	1:F:166:TYR:HA	1.57	0.45
1:F:363:LEU:HD12	1:F:363:LEU:HA	1.82	0.45
1:A:308:ASP:HA	1:A:312:LEU:HD13	1.97	0.45
1:A:362:LYS:HD2	4:C:624:HOH:O	2.15	0.45
1:A:369:THR:N	1:A:381:VAL:O	2.50	0.45
1:A:377:LEU:HD11	1:A:413:ARG:NH1	2.32	0.45
1:D:85:TYR:CD2	2:D:501:PLZ:H52	2.51	0.45
1:F:309:ASP:OD1	1:F:310:ILE:HG13	2.17	0.45
1:A:266:GLN:OE1	1:A:413:ARG:NH1	2.49	0.45
1:E:233:GLN:HB2	1:E:239:VAL:HB	1.99	0.45
1:F:158:TYR:HB3	1:F:165:LYS:HE3	1.98	0.45
1:B:178:TRP:CZ2	1:B:184:ALA:HA	2.52	0.45
1:D:266:GLN:HG3	4:D:615:HOH:O	2.16	0.45
1:D:282:ASN:ND2	1:E:284:ARG:NH2	2.64	0.45
1:E:294:LEU:HD23	1:E:301:VAL:HG12	1.98	0.45
1:A:255:ARG:HD3	4:A:628:HOH:O	2.17	0.44
1:C:381:VAL:HG22	1:C:411:ILE:HD12	2.00	0.44
1:D:214:ALA:HB3	4:D:620:HOH:O	2.18	0.44
1:D:119:VAL:CG2	1:D:327:PRO:HA	2.47	0.44
1:E:86:SER:O	1:E:293:ALA:HB2	2.17	0.44
1:E:178:TRP:CZ2	1:E:184:ALA:HA	2.52	0.44
1:C:345:LEU:HD13	1:C:418:LEU:HB2	1.99	0.44
1:C:299:TYR:HE2	1:C:326:ASN:HD21	1.64	0.44
1:F:292:LYS:HZ1	3:F:501:PLP:C3	2.31	0.44
1:A:361:MET:HE1	1:C:308:ASP:HB2	1.99	0.44
1:E:83:SER:HB3	4:E:630:HOH:O	2.18	0.44
1:F:426:ARG:O	1:F:430:GLU:HG2	2.16	0.44
1:B:340:LEU:HD23	1:B:345:LEU:HD12	1.99	0.44
1:C:120:LEU:O	1:C:124:GLU:HG3	2.18	0.44
1:A:258:VAL:HA	4:A:633:HOH:O	2.18	0.44
2:B:501:PLZ:H5M1	2:B:501:PLZ:HN9	1.83	0.44
1:A:178:TRP:CE2	1:A:184:ALA:HA	2.52	0.44
1:B:178:TRP:CE2	1:B:184:ALA:HA	2.53	0.44
1:C:93:CYS:SG	4:C:620:HOH:O	2.43	0.44
1:B:120:LEU:O	1:B:124:GLU:HG3	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:LEU:O	1:F:124:GLU:HG3	2.17	0.43
1:B:369:THR:N	1:B:381:VAL:O	2.49	0.43
1:F:246:LEU:HD13	1:F:278:VAL:HG12	2.00	0.43
1:A:434:LYS:N	4:A:619:HOH:O	2.51	0.43
1:B:362:LYS:NZ	4:B:664:HOH:O	2.47	0.43
1:E:41:ASP:O	1:E:45:GLU:HG2	2.17	0.43
1:E:97:ILE:HD12	1:E:97:ILE:H	1.82	0.43
1:A:138:PRO:HB2	4:A:693:HOH:O	2.18	0.43
1:A:340:LEU:HD23	1:A:345:LEU:HD12	2.00	0.43
1:C:363:LEU:HD22	1:C:436:ILE:HG21	2.00	0.43
1:D:38:PRO:HB2	1:D:43:ILE:CD1	2.48	0.43
1:E:120:LEU:O	1:E:124:GLU:HG3	2.19	0.43
1:F:321:SER:O	4:F:614:HOH:O	2.21	0.43
1:B:219:LEU:HD11	4:B:719:HOH:O	2.18	0.43
1:B:251:GLU:HG2	4:B:638:HOH:O	2.18	0.43
1:A:255:ARG:NE	1:A:255:ARG:HA	2.32	0.43
1:C:55:TYR:HH	1:C:180:ARG:NH2	2.16	0.43
1:E:406:PRO:O	4:E:617:HOH:O	2.21	0.43
1:A:434:LYS:O	1:A:438:SER:HB3	2.19	0.43
1:B:43:ILE:HD13	1:B:61:ALA:HB1	2.00	0.43
1:B:178:TRP:CD2	1:B:228:MET:HE1	2.54	0.43
1:D:357:ARG:O	1:D:361:MET:HG3	2.19	0.43
1:A:164:GLN:NE2	4:A:647:HOH:O	2.51	0.43
1:C:62:LEU:CD1	1:C:70:LEU:HD13	2.48	0.43
1:C:110:LEU:HD22	1:C:323:TYR:CE1	2.54	0.43
1:E:97:ILE:CD1	1:E:339:VAL:HG21	2.49	0.43
2:D:501:PLZ:O2	4:D:619:HOH:O	2.22	0.42
1:E:102:LYS:O	1:E:105:VAL:HG12	2.19	0.42
1:F:86:SER:O	1:F:293:ALA:HB2	2.18	0.42
1:F:97:ILE:H	1:F:97:ILE:HD12	1.83	0.42
1:C:343:GLU:OE2	4:C:621:HOH:O	2.21	0.42
1:E:292:LYS:HE3	1:F:322:THR:HG21	2.00	0.42
1:F:265:ILE:HG22	1:F:292:LYS:NZ	2.34	0.42
1:F:369:THR:N	1:F:381:VAL:O	2.52	0.42
1:A:299:TYR:HE2	1:A:326:ASN:HD21	1.67	0.42
1:B:221:ASP:HB3	1:B:224:VAL:HG23	2.00	0.42
1:F:438:SER:N	4:F:605:HOH:O	2.52	0.42
1:A:85:TYR:CE2	2:A:501:PLZ:H62	2.54	0.42
1:E:154:ARG:NH1	1:F:199:PRO:O	2.52	0.42
1:E:342:GLU:HG3	1:E:343:GLU:N	2.34	0.42
1:A:423:ASP:O	1:A:426:ARG:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:VAL:HG23	1:D:179:GLY:HA3	2.02	0.42
1:F:68:ILE:HD11	4:F:607:HOH:O	2.19	0.42
1:F:374:LYS:HA	1:F:374:LYS:HD2	1.78	0.42
1:C:43:ILE:HD13	1:C:61:ALA:HB1	2.01	0.42
1:C:364:PRO:HG2	1:C:367:VAL:HG22	2.00	0.42
1:E:299:TYR:CZ	1:F:300:PRO:HD3	2.55	0.42
1:B:110:LEU:HD22	1:B:112:SER:H	1.84	0.42
1:B:235:GLU:HG3	4:B:617:HOH:O	2.18	0.42
1:E:64:ARG:HB3	1:E:71:TRP:HB2	2.02	0.42
1:A:216:GLU:HB3	4:A:645:HOH:O	2.20	0.41
1:D:117:ASN:ND2	1:D:327:PRO:HD3	2.34	0.41
1:D:421:LYS:HE3	1:D:421:LYS:HB3	1.91	0.41
1:A:70:LEU:HD21	1:A:92:HIS:CE1	2.55	0.41
1:F:37:PRO:HA	1:F:38:PRO:HD3	1.91	0.41
1:F:58:LEU:O	1:F:60:VAL:N	2.53	0.41
1:F:390:ALA:HB1	1:F:412:ILE:HG12	2.02	0.41
1:A:120:LEU:O	1:A:124:GLU:HG3	2.20	0.41
1:B:250:ARG:HB2	1:B:283:VAL:HG23	2.01	0.41
1:C:301:VAL:HG22	4:C:638:HOH:O	2.20	0.41
1:A:426:ARG:O	1:A:427:GLU:CB	2.68	0.41
1:C:58:LEU:O	1:C:60:VAL:N	2.53	0.41
1:E:113:ARG:O	4:E:618:HOH:O	2.21	0.41
1:A:221:ASP:HB3	1:A:224:VAL:HG23	2.01	0.41
1:B:407:THR:HB	1:B:411:ILE:HB	2.01	0.41
1:B:410:ASP:N	4:B:613:HOH:O	2.52	0.41
1:C:64:ARG:NH2	1:C:66:LYS:HD3	2.35	0.41
1:B:86:SER:O	1:B:293:ALA:HB2	2.21	0.41
1:C:427:GLU:OE2	4:C:622:HOH:O	2.21	0.41
1:D:110:LEU:HD22	1:D:323:TYR:CE2	2.56	0.41
1:A:405:LYS:NZ	1:A:413:ARG:HE	2.19	0.41
1:B:230:GLU:OE1	1:B:233:GLN:HA	2.19	0.41
1:D:49:LYS:HE3	1:D:50:TYR:OH	2.21	0.41
1:E:104:GLN:HB2	1:E:331:ARG:HG3	2.03	0.41
1:E:367:VAL:HG22	1:E:388:TRP:CH2	2.55	0.41
1:A:424:GLU:HG2	4:A:626:HOH:O	2.20	0.41
1:C:55:TYR:OH	1:C:180:ARG:NH2	2.54	0.41
1:C:144:GLU:CD	4:C:641:HOH:O	2.64	0.41
1:D:103:SER:HB3	4:D:668:HOH:O	2.21	0.41
1:F:101:LEU:HD13	1:F:298:LEU:HD23	2.02	0.41
1:F:139:MET:HE1	1:F:321:SER:HB2	2.03	0.41
1:F:209:TYR:CZ	1:F:233:GLN:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:GLN:CD	4:F:631:HOH:O	2.64	0.41
1:E:178:TRP:CE2	1:E:184:ALA:HA	2.55	0.41
1:E:212:LEU:N	1:E:213:PRO:CD	2.83	0.41
1:B:58:LEU:O	1:B:60:VAL:N	2.54	0.40
1:C:265:ILE:HG23	1:C:292:LYS:HD3	2.01	0.40
1:D:58:LEU:O	1:D:60:VAL:N	2.54	0.40
1:C:86:SER:O	1:C:293:ALA:HB2	2.22	0.40
1:E:155:LYS:HD3	1:F:197:PHE:CE1	2.56	0.40
1:A:233:GLN:HB2	1:A:239:VAL:HB	2.03	0.40
1:C:64:ARG:HH22	1:C:66:LYS:HD3	1.85	0.40
1:C:123:TYR:HB2	1:C:334:ILE:HD11	2.03	0.40
1:D:357:ARG:HA	4:D:703:HOH:O	2.22	0.40
1:F:110:LEU:HD22	1:F:323:TYR:CE2	2.56	0.40
1:D:233:GLN:HB2	1:D:239:VAL:HB	2.02	0.40
1:D:369:THR:N	1:D:381:VAL:O	2.51	0.40
1:A:434:LYS:HD3	1:A:434:LYS:C	2.46	0.40
1:C:366:ASP:OD1	1:C:367:VAL:HG13	2.21	0.40
1:D:276:LEU:HB3	1:D:278:VAL:HG22	2.03	0.40
1:D:413:ARG:N	4:D:611:HOH:O	2.54	0.40
1:E:199:PRO:O	1:F:154:ARG:NH1	2.52	0.40

All (13) 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)
4:B:761:HOH:O	4:D:731:HOH:O[4_456]	1.87	0.33
4:A:681:HOH:O	4:D:691:HOH:O[4_566]	1.96	0.24
4:A:654:HOH:O	4:F:635:HOH:O[5_675]	2.02	0.18
4:C:627:HOH:O	4:C:679:HOH:O[5_675]	2.02	0.18
4:B:641:HOH:O	4:B:724:HOH:O[4_466]	2.03	0.17
1:C:366:ASP:OD2	1:F:102:LYS:NZ[5_565]	2.09	0.11
4:A:690:HOH:O	4:D:669:HOH:O[4_566]	2.12	0.08
4:A:658:HOH:O	4:D:640:HOH:O[4_566]	2.13	0.07
4:B:636:HOH:O	4:B:651:HOH:O[4_466]	2.13	0.07
4:B:699:HOH:O	4:B:763:HOH:O[4_466]	2.13	0.07
1:A:165:LYS:NZ	1:D:195:ASP:OD1[4_566]	2.14	0.06
4:B:637:HOH:O	4:E:724:HOH:O[4_456]	2.14	0.06
1:C:64:ARG:NH1	1:C:107:LYS:O[5_675]	2.17	0.03

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	402/439 (92%)	380 (94%)	21 (5%)	1 (0%)	43	51
1	B	402/439 (92%)	382 (95%)	19 (5%)	1 (0%)	43	51
1	C	402/439 (92%)	382 (95%)	20 (5%)	0	100	100
1	D	400/439 (91%)	379 (95%)	20 (5%)	1 (0%)	36	42
1	E	402/439 (92%)	381 (95%)	21 (5%)	0	100	100
1	F	401/439 (91%)	380 (95%)	20 (5%)	1 (0%)	43	51
All	All	2409/2634 (92%)	2284 (95%)	121 (5%)	4 (0%)	43	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	GLU
1	F	59	PRO
1	B	59	PRO
1	D	59	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/366 (92%)	324 (96%)	13 (4%)	28	39
1	B	337/366 (92%)	326 (97%)	11 (3%)	33	45
1	C	337/366 (92%)	333 (99%)	4 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	336/366 (92%)	326 (97%)	10 (3%)	36	49
1	E	337/366 (92%)	326 (97%)	11 (3%)	33	45
1	F	337/366 (92%)	330 (98%)	7 (2%)	47	63
All	All	2021/2196 (92%)	1965 (97%)	56 (3%)	38	52

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	112	SER
1	A	130	LEU
1	A	171	VAL
1	A	180	ARG
1	A	255	ARG
1	A	283	VAL
1	A	344	ASN
1	A	371	VAL
1	A	386	LYS
1	A	428	SER
1	A	434	LYS
1	A	437	LEU
1	B	110	LEU
1	B	111	THR
1	B	112	SER
1	B	130	LEU
1	B	152	LEU
1	B	193	SER
1	B	251	GLU
1	B	358	ASN
1	B	361	MET
1	B	366	ASP
1	B	428	SER
1	C	112	SER
1	C	292	LYS
1	C	376	LEU
1	C	428	SER
1	D	43	ILE
1	D	111	THR
1	D	112	SER
1	D	119	VAL
1	D	235	GLU

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Mol	Chain	Res	Type
1	D	266	GLN
1	D	371	VAL
1	D	407	THR
1	D	413	ARG
1	D	428	SER
1	E	112	SER
1	E	165	LYS
1	E	223	ASN
1	E	235	GLU
1	E	334	ILE
1	E	369	THR
1	E	371	VAL
1	E	376	LEU
1	E	407	THR
1	E	425	LEU
1	E	428	SER
1	F	45	GLU
1	F	112	SER
1	F	165	LYS
1	F	341	GLU
1	F	363	LEU
1	F	369	THR
1	F	428	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	ASN
1	B	164	GLN
1	B	344	ASN
1	D	282	ASN
1	E	140	ASN
1	F	266	GLN

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$
2	PLZ	C	501	-	22,22,22	2.52	9 (40%)	29,30,30	2.19	7 (24%)
2	PLZ	A	501	-	22,22,22	2.32	7 (31%)	29,30,30	1.94	6 (20%)
2	PLZ	B	501	-	22,22,22	2.48	9 (40%)	29,30,30	2.96	7 (24%)
3	PLP	F	501	-	15,15,16	1.06	1 (6%)	21,22,23	0.97	2 (9%)
3	PLP	E	501	-	15,15,16	1.12	1 (6%)	21,22,23	1.04	2 (9%)
2	PLZ	D	501	-	22,22,22	2.50	7 (31%)	29,30,30	1.76	5 (17%)

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
2	PLZ	C	501	-	-	3/14/14/14	0/1/1/1
2	PLZ	A	501	-	-	3/14/14/14	0/1/1/1
2	PLZ	B	501	-	-	7/14/14/14	0/1/1/1
3	PLP	F	501	-	-	0/6/6/8	0/1/1/1
3	PLP	E	501	-	-	3/6/6/8	0/1/1/1
2	PLZ	D	501	-	-	5/14/14/14	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLZ	C8-N9	-6.15	1.26	1.47
2	A	501	PLZ	C8-N9	-6.00	1.27	1.47
2	A	501	PLZ	C2A-C12	5.99	1.59	1.50
2	D	501	PLZ	C2A-C12	5.96	1.59	1.50
2	B	501	PLZ	C8-N9	-5.96	1.27	1.47
2	D	501	PLZ	C8-N9	-5.94	1.27	1.47
2	B	501	PLZ	C2A-C12	5.92	1.59	1.50
2	C	501	PLZ	C2A-C12	5.89	1.59	1.50
2	D	501	PLZ	P-O2P	4.40	1.64	1.50
2	C	501	PLZ	P-O2P	3.66	1.61	1.50
2	B	501	PLZ	P-O2P	3.64	1.61	1.50
2	C	501	PLZ	P-O4P	2.97	1.69	1.60
2	B	501	PLZ	C13-C12	-2.93	1.37	1.41
2	C	501	PLZ	C5M-C15	2.90	1.58	1.50
2	D	501	PLZ	P-O4P	2.89	1.69	1.60
2	A	501	PLZ	P-O4P	2.87	1.69	1.60
2	B	501	PLZ	P-O4P	2.86	1.69	1.60
2	D	501	PLZ	C6-C1	2.76	1.57	1.50
2	B	501	PLZ	C5M-C15	2.71	1.58	1.50
2	A	501	PLZ	C5M-C15	2.69	1.57	1.50
2	D	501	PLZ	C5M-C15	2.66	1.57	1.50
2	C	501	PLZ	C13-C12	-2.61	1.38	1.41
3	E	501	PLP	C2-N1	2.60	1.38	1.33
2	A	501	PLZ	C6-C1	2.56	1.56	1.50
3	F	501	PLP	C2-N1	2.54	1.38	1.33
2	C	501	PLZ	P-O3P	2.46	1.64	1.54
2	C	501	PLZ	C6-C1	2.45	1.56	1.50
2	A	501	PLZ	P-O1P	2.43	1.63	1.54
2	B	501	PLZ	P-O3P	2.43	1.63	1.54
2	D	501	PLZ	O3-C13	2.38	1.42	1.36
2	B	501	PLZ	O3-C13	2.30	1.42	1.36
2	B	501	PLZ	C6-C1	2.28	1.55	1.50
2	A	501	PLZ	O3-C13	2.23	1.42	1.36
2	C	501	PLZ	O3-C13	2.05	1.41	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLZ	C4A-C19-C15	10.00	130.64	119.75
2	C	501	PLZ	C4A-C19-C15	7.36	127.76	119.75
2	B	501	PLZ	C4A-C19-C13	-6.72	111.05	119.98
2	B	501	PLZ	C19-C4A-N9	6.17	122.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLZ	C5-C8-N9	4.90	125.24	112.07
2	A	501	PLZ	C19-C4A-N9	4.74	120.25	111.50
2	B	501	PLZ	C2A-C12-C13	-4.53	115.49	120.80
2	D	501	PLZ	C5-C8-N9	4.33	123.69	112.07
2	C	501	PLZ	C4A-C19-C13	-4.23	114.36	119.98
2	C	501	PLZ	C2A-C12-C13	-4.01	116.10	120.80
2	D	501	PLZ	C19-C4A-N9	3.98	118.84	111.50
2	B	501	PLZ	C5-C8-N9	3.89	122.51	112.07
2	A	501	PLZ	C4A-C19-C13	3.48	124.61	119.98
2	D	501	PLZ	C4A-C19-C13	3.18	124.21	119.98
2	D	501	PLZ	C16-C15-C19	3.15	120.45	118.06
2	B	501	PLZ	C2A-C12-N1	3.09	123.47	117.64
2	C	501	PLZ	C19-C4A-N9	3.01	117.06	111.50
2	A	501	PLZ	C4A-C19-C15	-2.94	116.55	119.75
2	A	501	PLZ	C16-C15-C19	2.70	120.10	118.06
2	B	501	PLZ	C5-C6-C1	-2.65	107.59	114.51
2	A	501	PLZ	C15-C16-N1	-2.64	119.54	123.83
2	C	501	PLZ	C2A-C12-N1	2.60	122.54	117.64
2	C	501	PLZ	O4P-C5M-C15	2.54	114.11	109.36
2	D	501	PLZ	C15-C16-N1	-2.44	119.87	123.83
2	C	501	PLZ	C5-C8-N9	2.33	118.32	112.07
3	F	501	PLP	C6-C5-C4	2.28	119.97	118.10
3	E	501	PLP	C5-C6-N1	-2.24	120.18	123.83
3	F	501	PLP	C5-C6-N1	-2.21	120.24	123.83
3	E	501	PLP	C6-C5-C4	2.12	119.84	118.10

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLZ	C13-C19-C4A-N9
2	B	501	PLZ	C15-C19-C4A-N9
2	B	501	PLZ	C19-C15-C5M-O4P
2	C	501	PLZ	C13-C19-C4A-N9
2	C	501	PLZ	C15-C19-C4A-N9
2	D	501	PLZ	C15-C19-C4A-N9
3	E	501	PLP	C5A-O4P-P-O1P
3	E	501	PLP	C5A-O4P-P-O2P
2	A	501	PLZ	C15-C19-C4A-N9
2	B	501	PLZ	C6-C5-C8-N9
2	D	501	PLZ	C6-C5-C8-N9
2	A	501	PLZ	C6-C5-C8-N9

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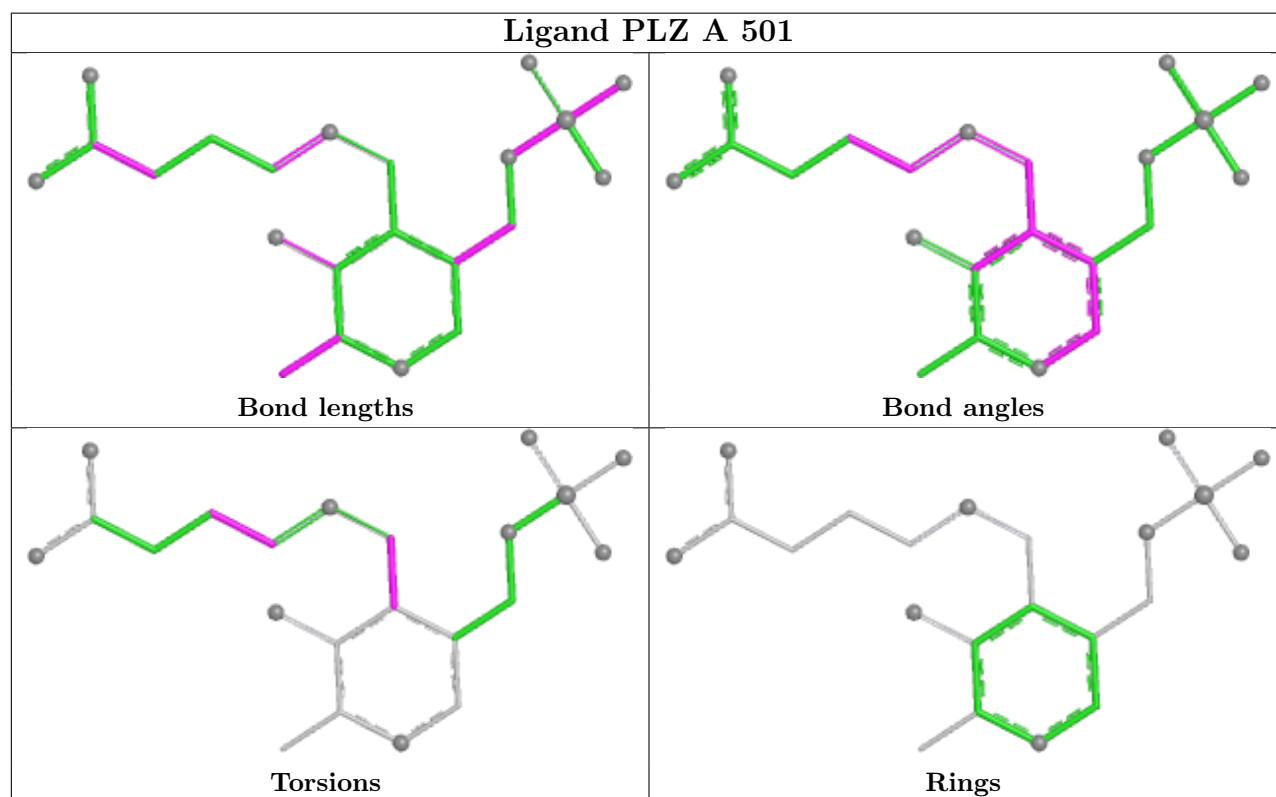
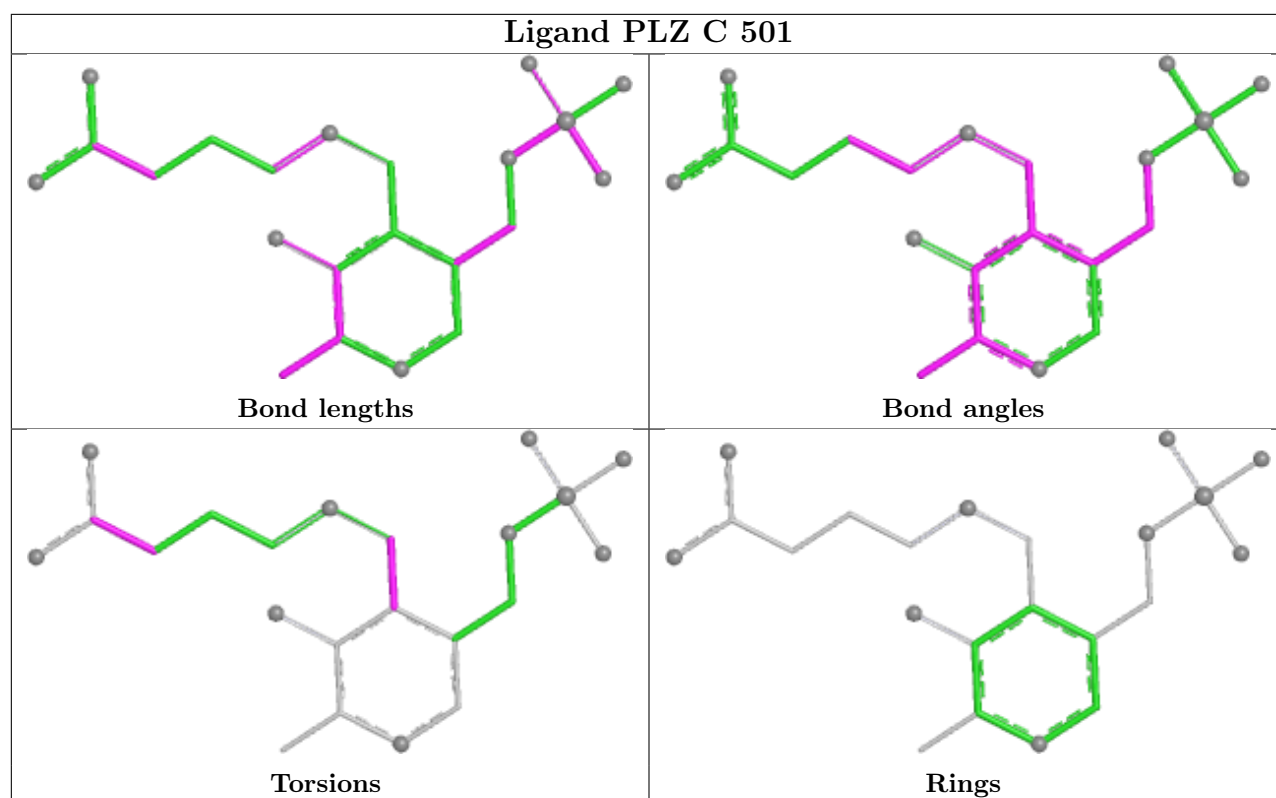
Mol	Chain	Res	Type	Atoms
2	D	501	PLZ	C13-C19-C4A-N9
2	A	501	PLZ	C13-C19-C4A-N9
2	B	501	PLZ	C16-C15-C5M-O4P
2	B	501	PLZ	O4-C1-C6-C5
2	B	501	PLZ	O2-C1-C6-C5
2	D	501	PLZ	O2-C1-C6-C5
3	E	501	PLP	C5A-O4P-P-O3P
2	D	501	PLZ	O4-C1-C6-C5
2	C	501	PLZ	O2-C1-C6-C5

There are no ring outliers.

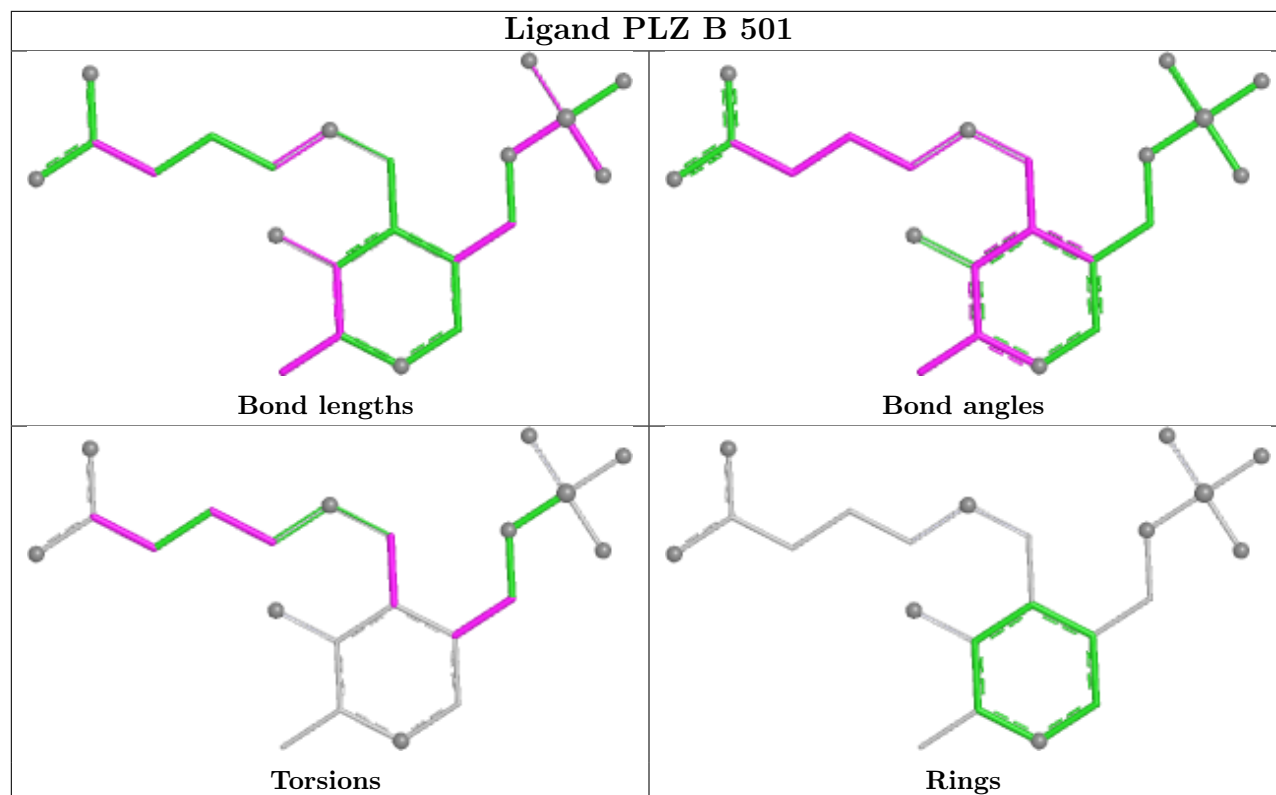
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PLZ	3	0
2	A	501	PLZ	3	0
2	B	501	PLZ	1	0
3	F	501	PLP	1	0
3	E	501	PLP	1	0
2	D	501	PLZ	2	0

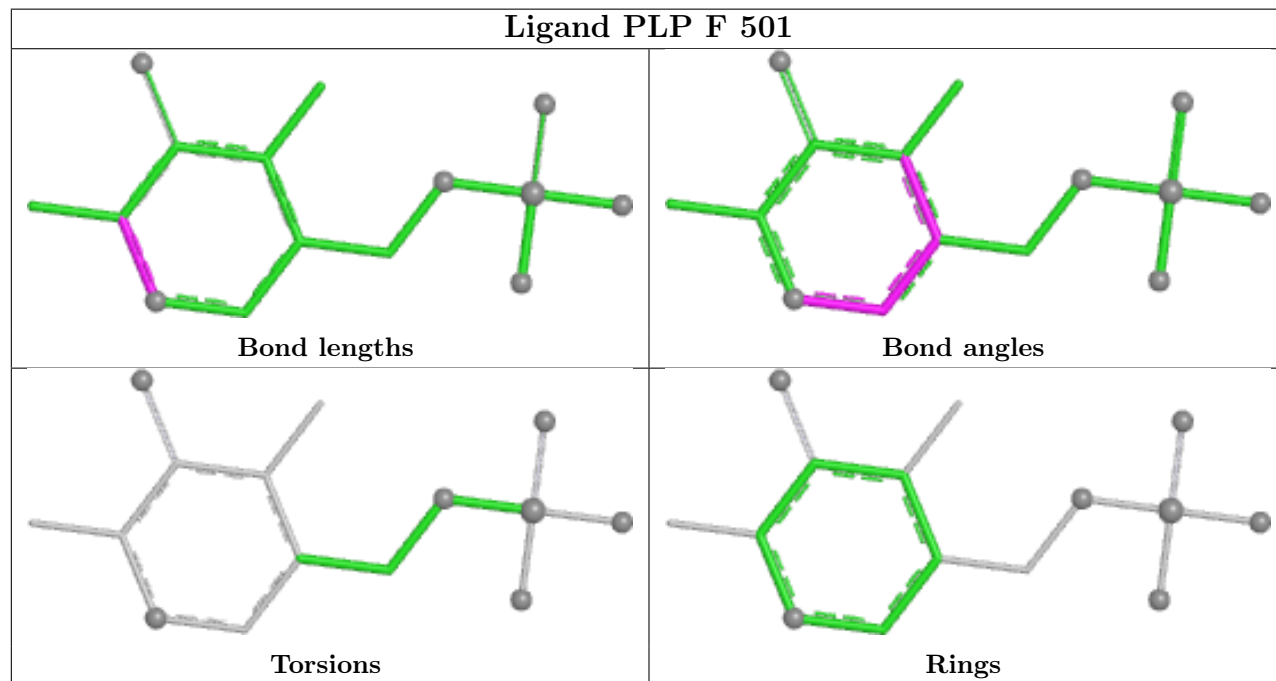
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

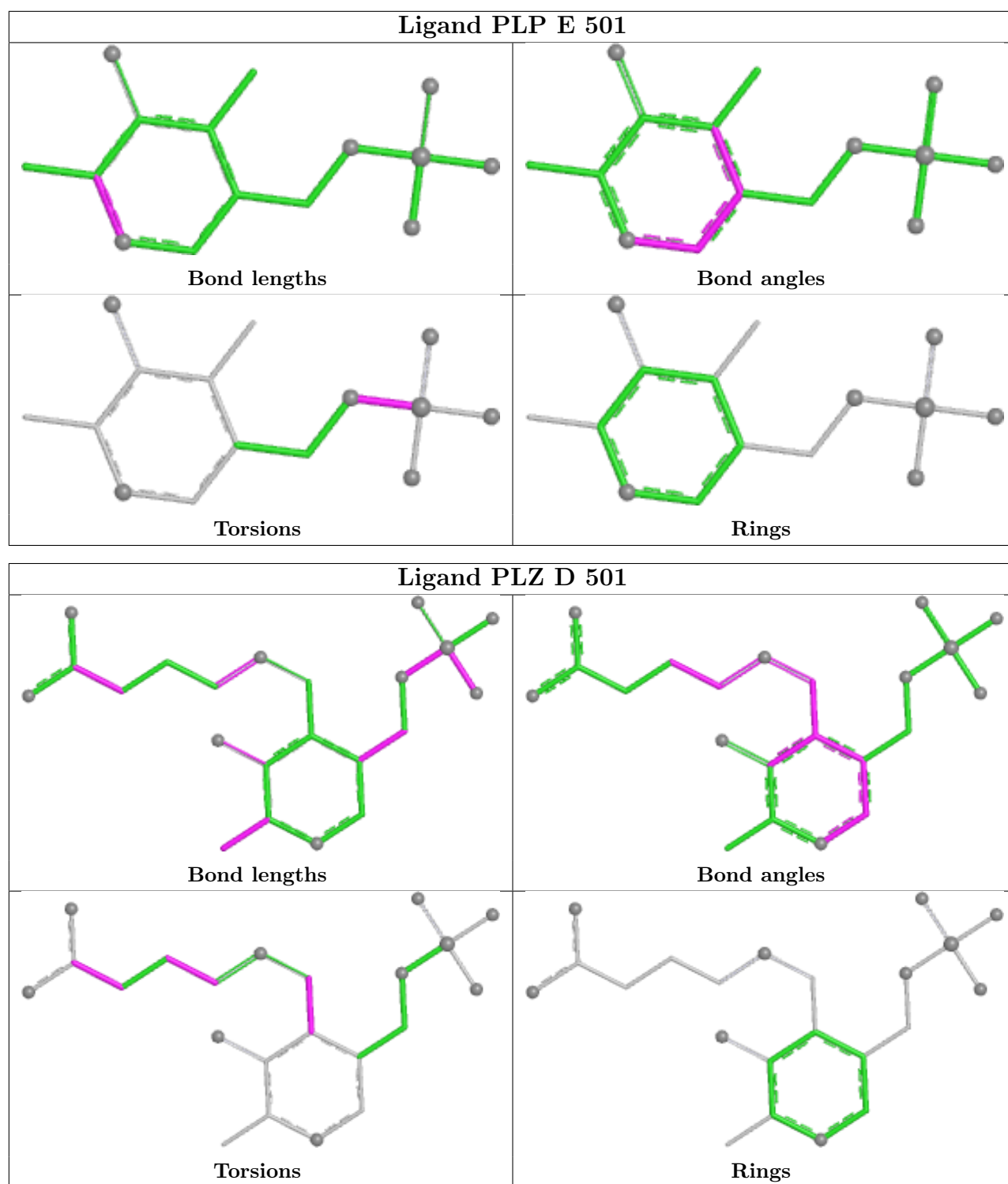


Ligand PLZ B 501



Ligand PLP F 501





5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/439 (92%)	-0.52	0 100 100	31, 42, 55, 72	0
1	B	404/439 (92%)	-0.61	0 100 100	26, 36, 49, 61	0
1	C	404/439 (92%)	-0.54	0 100 100	27, 40, 52, 62	0
1	D	402/439 (91%)	-0.50	0 100 100	30, 42, 53, 64	0
1	E	404/439 (92%)	-0.64	0 100 100	28, 38, 51, 70	0
1	F	403/439 (91%)	-0.61	0 100 100	26, 38, 52, 64	0
All	All	2421/2634 (91%)	-0.57	0 100 100	26, 39, 53, 72	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PLP	F	501	15/16	0.97	0.08	18,26,31,34	0

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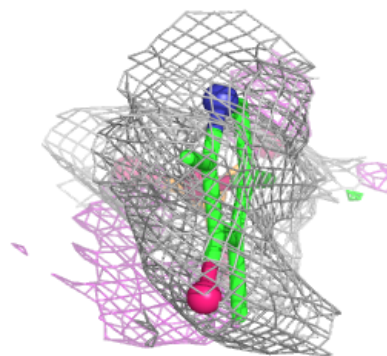
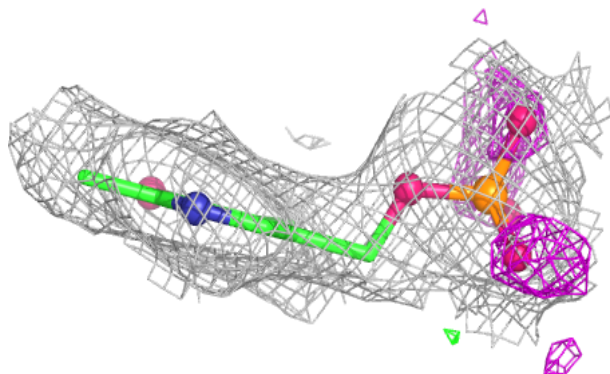
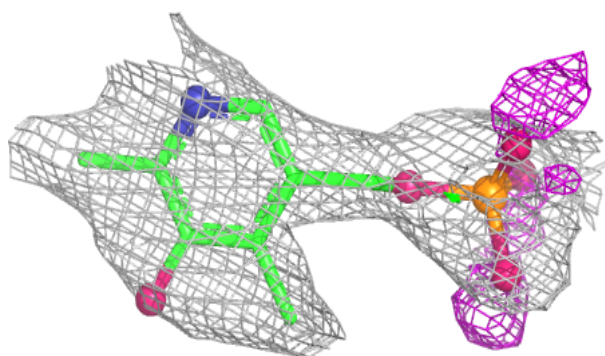
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLZ	C	501	22/22	0.98	0.05	23,25,28,32	0
3	PLP	E	501	15/16	0.98	0.05	15,21,23,25	0
2	PLZ	B	501	22/22	0.98	0.05	16,25,33,38	0
2	PLZ	A	501	22/22	0.99	0.05	15,23,31,32	0
2	PLZ	D	501	22/22	0.99	0.05	15,26,36,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

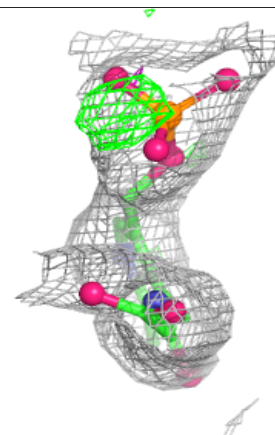
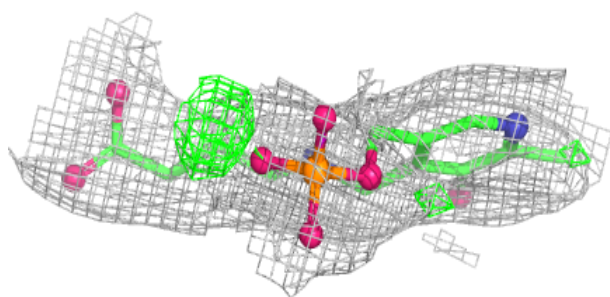
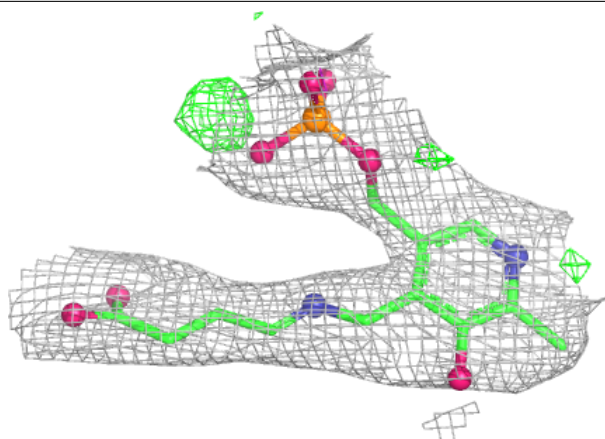
Electron density around PLP F 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

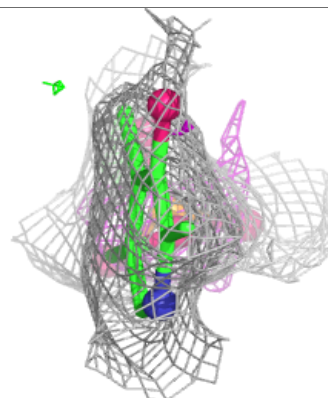
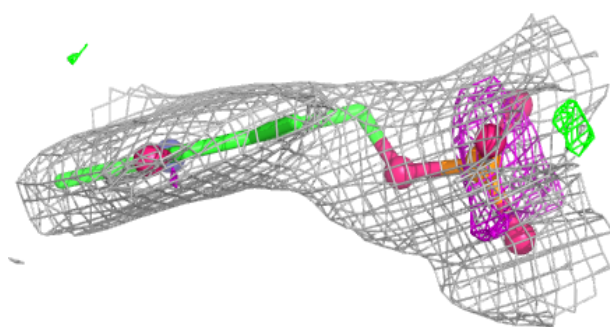
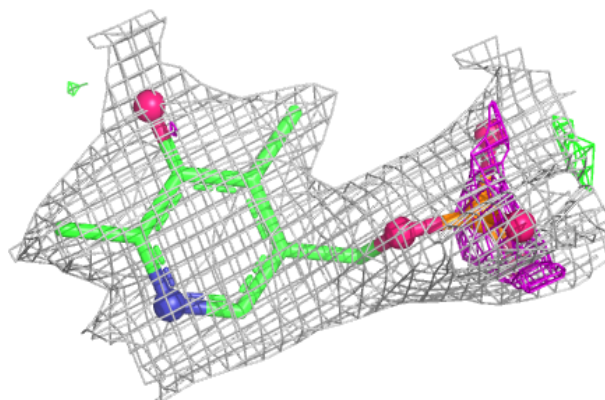


Electron density around PLZ C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

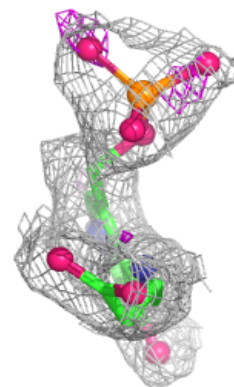
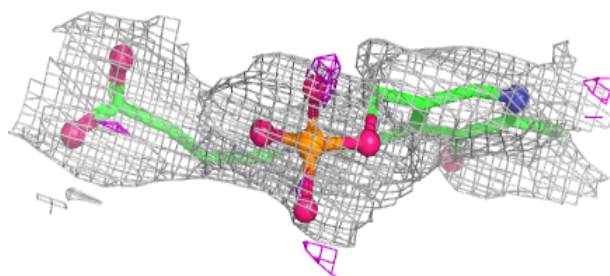
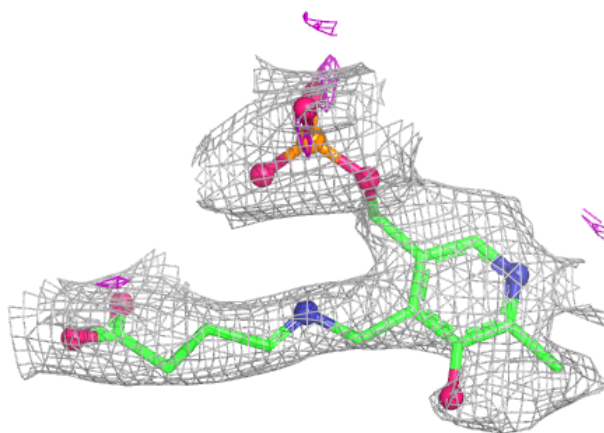
**Electron density around PLP E 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

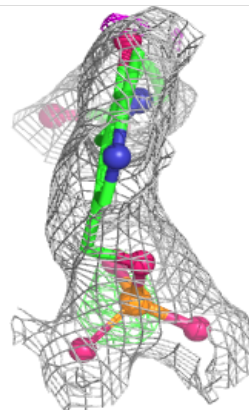
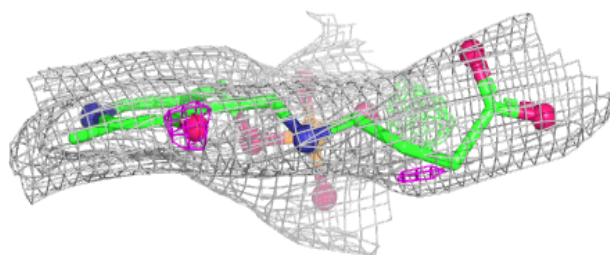
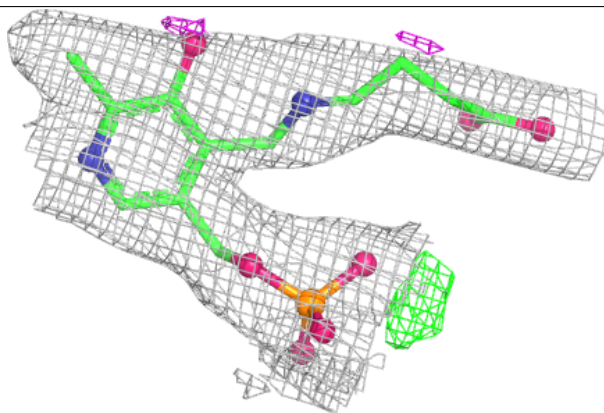


Electron density around PLZ B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

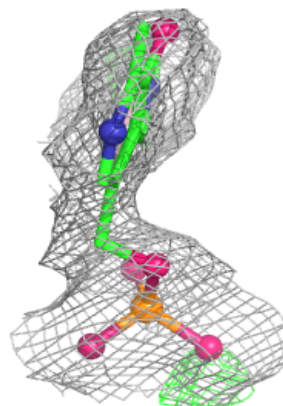
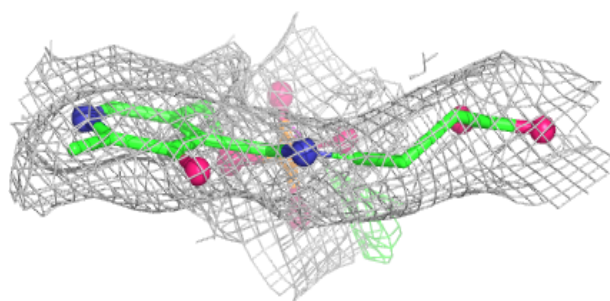
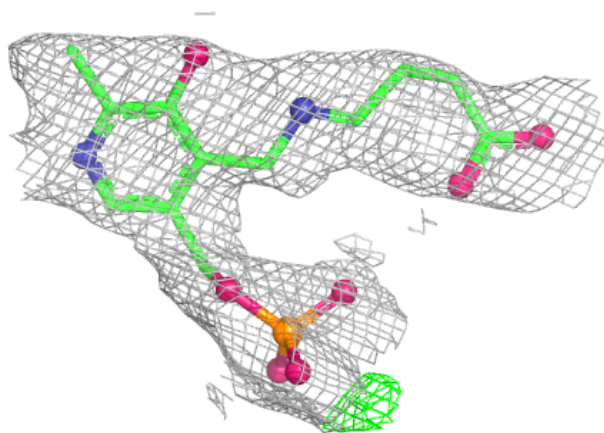
**Electron density around PLZ A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLZ D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.