



Full wwPDB X-ray Structure Validation Report i

Dec 8, 2021 – 02:08 pm GMT

PDB ID : 7P3T
Title : Transaminase of gamma-proteobacterium
Authors : Ermler, U.
Deposited on : 2021-07-08
Resolution : 1.60 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 i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

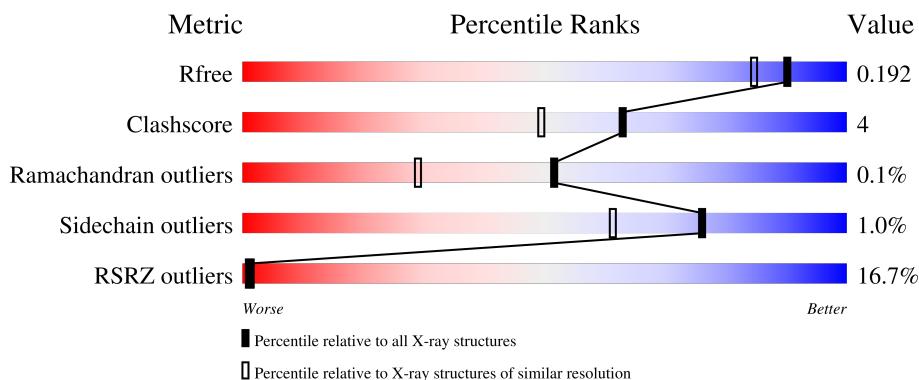
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

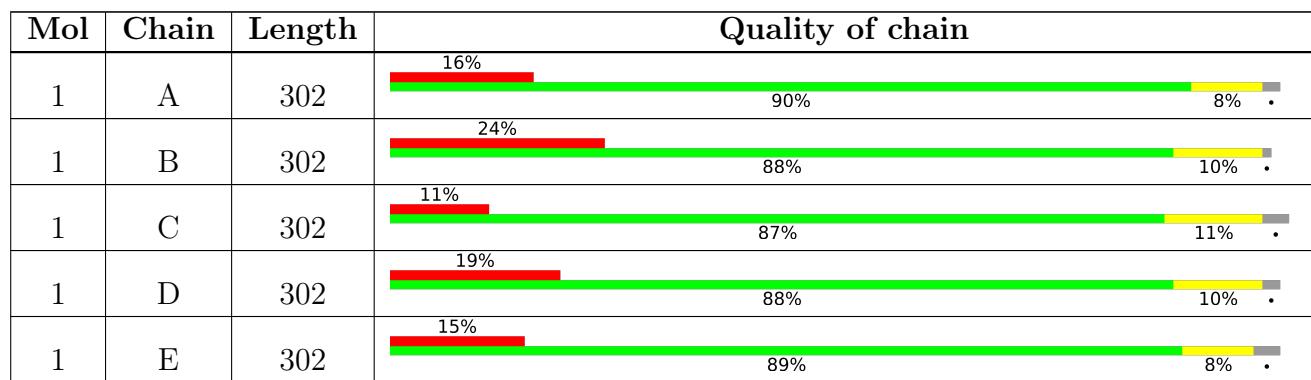
The reported resolution of this entry is 1.60 Å.

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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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.



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Mol	Chain	Length	Quality of chain	
1	F	302	15%	91% 6% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15759 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 Branched-chain amino acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total 2359	C 1493	N 416	O 443	S 7	0	3	0
1	B	299	Total 2429	C 1533	N 439	O 451	S 6	0	7	0
1	C	294	Total 2426	C 1529	N 432	O 459	S 6	0	12	0
1	D	295	Total 2382	C 1505	N 424	O 447	S 6	0	6	0
1	E	294	Total 2397	C 1514	N 430	O 447	S 6	0	8	0
1	F	294	Total 2367	C 1498	N 416	O 447	S 6	0	6	0

There are 54 discrepancies between the modelled and reference sequences:

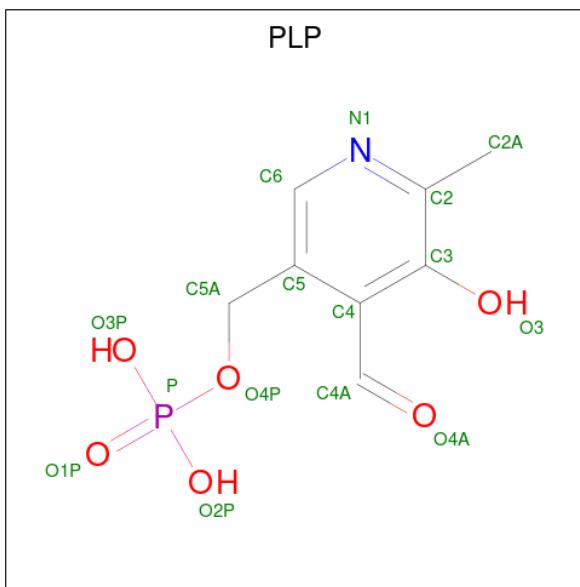
Chain	Residue	Modelled	Actual	Comment	Reference
A	294	SER	-	expression tag	UNP B8KQT8
A	295	GLY	-	expression tag	UNP B8KQT8
A	296	SER	-	expression tag	UNP B8KQT8
A	297	HIS	-	expression tag	UNP B8KQT8
A	298	HIS	-	expression tag	UNP B8KQT8
A	299	HIS	-	expression tag	UNP B8KQT8
A	300	HIS	-	expression tag	UNP B8KQT8
A	301	HIS	-	expression tag	UNP B8KQT8
A	302	HIS	-	expression tag	UNP B8KQT8
B	294	SER	-	expression tag	UNP B8KQT8
B	295	GLY	-	expression tag	UNP B8KQT8
B	296	SER	-	expression tag	UNP B8KQT8
B	297	HIS	-	expression tag	UNP B8KQT8
B	298	HIS	-	expression tag	UNP B8KQT8
B	299	HIS	-	expression tag	UNP B8KQT8
B	300	HIS	-	expression tag	UNP B8KQT8
B	301	HIS	-	expression tag	UNP B8KQT8

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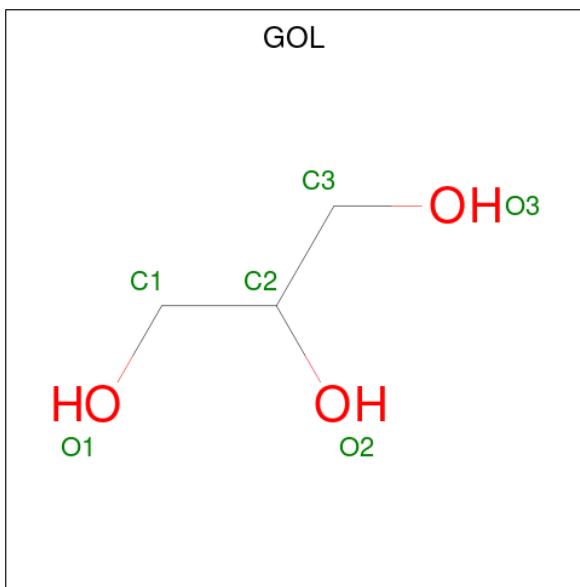
Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP B8KQT8
C	294	SER	-	expression tag	UNP B8KQT8
C	295	GLY	-	expression tag	UNP B8KQT8
C	296	SER	-	expression tag	UNP B8KQT8
C	297	HIS	-	expression tag	UNP B8KQT8
C	298	HIS	-	expression tag	UNP B8KQT8
C	299	HIS	-	expression tag	UNP B8KQT8
C	300	HIS	-	expression tag	UNP B8KQT8
C	301	HIS	-	expression tag	UNP B8KQT8
C	302	HIS	-	expression tag	UNP B8KQT8
D	294	SER	-	expression tag	UNP B8KQT8
D	295	GLY	-	expression tag	UNP B8KQT8
D	296	SER	-	expression tag	UNP B8KQT8
D	297	HIS	-	expression tag	UNP B8KQT8
D	298	HIS	-	expression tag	UNP B8KQT8
D	299	HIS	-	expression tag	UNP B8KQT8
D	300	HIS	-	expression tag	UNP B8KQT8
D	301	HIS	-	expression tag	UNP B8KQT8
D	302	HIS	-	expression tag	UNP B8KQT8
E	294	SER	-	expression tag	UNP B8KQT8
E	295	GLY	-	expression tag	UNP B8KQT8
E	296	SER	-	expression tag	UNP B8KQT8
E	297	HIS	-	expression tag	UNP B8KQT8
E	298	HIS	-	expression tag	UNP B8KQT8
E	299	HIS	-	expression tag	UNP B8KQT8
E	300	HIS	-	expression tag	UNP B8KQT8
E	301	HIS	-	expression tag	UNP B8KQT8
E	302	HIS	-	expression tag	UNP B8KQT8
F	294	SER	-	expression tag	UNP B8KQT8
F	295	GLY	-	expression tag	UNP B8KQT8
F	296	SER	-	expression tag	UNP B8KQT8
F	297	HIS	-	expression tag	UNP B8KQT8
F	298	HIS	-	expression tag	UNP B8KQT8
F	299	HIS	-	expression tag	UNP B8KQT8
F	300	HIS	-	expression tag	UNP B8KQT8
F	301	HIS	-	expression tag	UNP B8KQT8
F	302	HIS	-	expression tag	UNP B8KQT8

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total		C	N	O	P	
			15	8	1	5	1		
2	B	1	Total		C	N	O	P	
			15	8	1	5	1		
2	C	1	Total		C	N	O	P	
			15	8	1	5	1		
2	D	1	Total		C	N	O	P	
			15	8	1	5	1		
2	E	1	Total		C	N	O	P	
			15	8	1	5	1		
2	F	1	Total		C	N	O	P	
			15	8	1	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

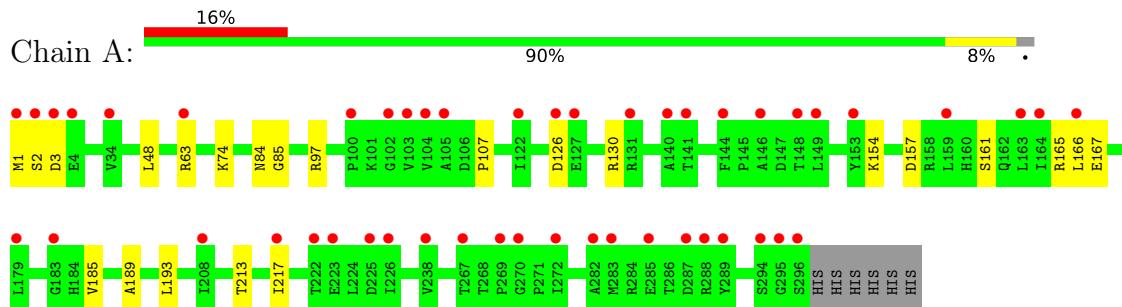
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	221	Total O 223 223	0	2
4	B	210	Total O 212 212	0	2
4	C	253	Total O 254 254	0	1
4	D	183	Total O 186 186	0	3
4	E	181	Total O 182 182	0	1
4	F	215	Total O 216 216	0	1

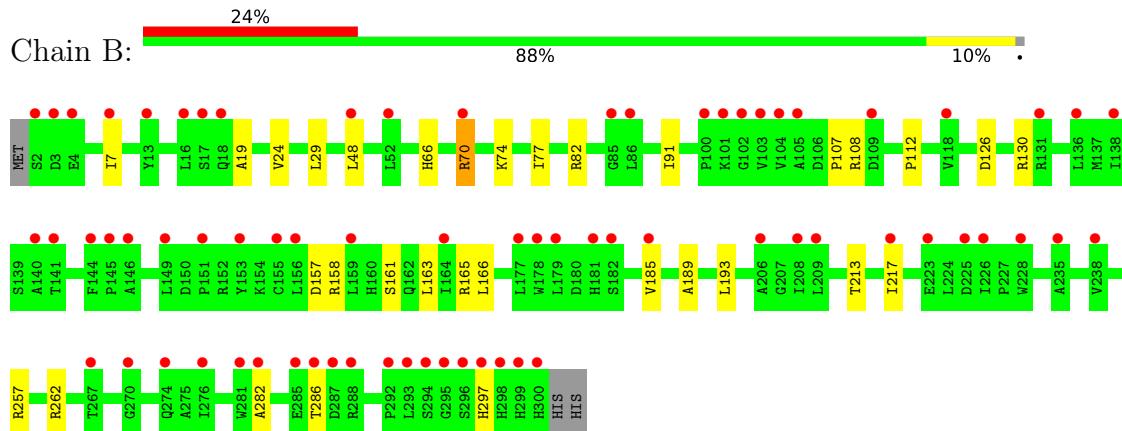
3 Residue-property plots [i](#)

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.

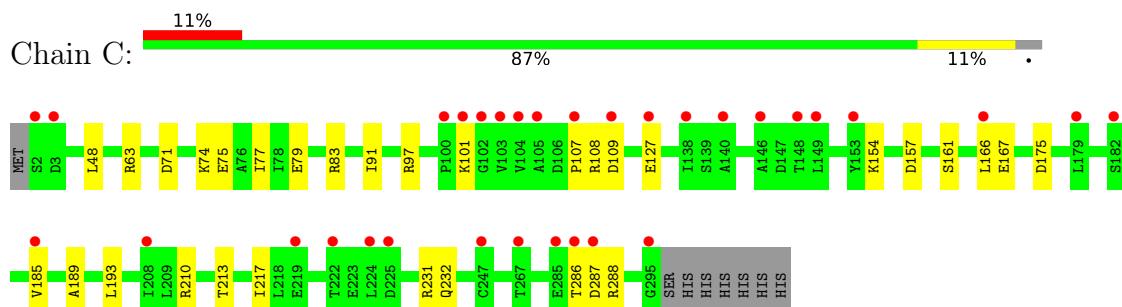
- Molecule 1: Branched-chain amino acid aminotransferase



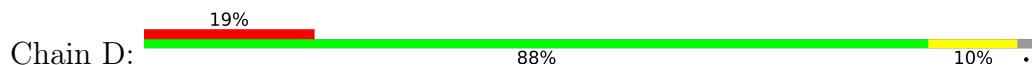
- Molecule 1: Branched-chain amino acid aminotransferase

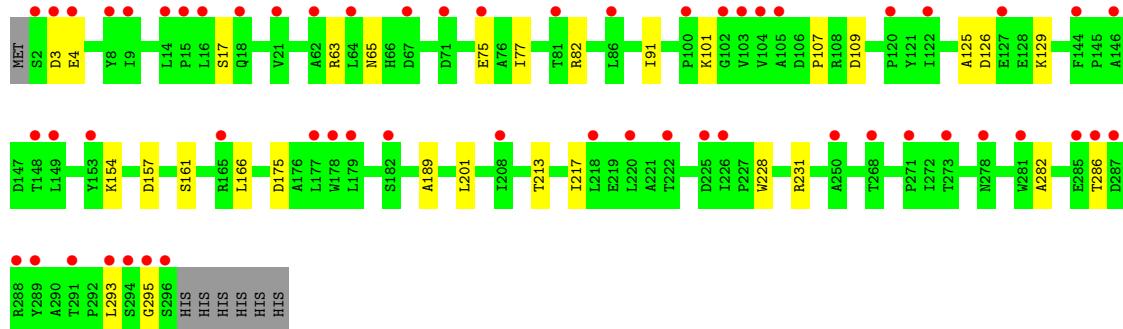


- Molecule 1: Branched-chain amino acid aminotransferase



- Molecule 1: Branched-chain amino acid aminotransferase

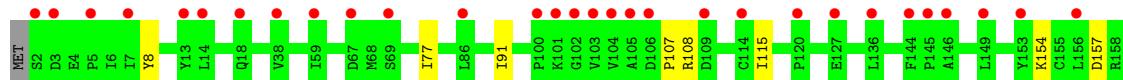




- Molecule 1: Branched-chain amino acid aminotransferase



- Molecule 1: Branched-chain amino acid aminotransferase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.81 Å 144.58 Å 151.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.93 – 1.60 45.93 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.93-1.60) 99.7 (45.93-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.45 (at 1.60 Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R , R_{free}	0.169 , 0.185 0.176 , 0.192	Depositor DCC
R_{free} test set	12305 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15759	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: PLP, GOL

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	0.46	0/2412	0.66	0/3278
1	B	0.38	0/2487	0.64	0/3379
1	C	0.43	0/2479	0.66	0/3367
1	D	0.40	0/2435	0.64	0/3308
1	E	0.38	0/2451	0.62	0/3329
1	F	0.41	0/2420	0.63	0/3289
All	All	0.41	0/14684	0.64	0/19950

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 [\(i\)](#)

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	2359	0	2322	28	0
1	B	2429	0	2373	27	0
1	C	2426	0	2369	33	0
1	D	2382	0	2339	22	0
1	E	2397	0	2353	17	0
1	F	2367	0	2321	18	0
2	A	15	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
2	E	15	0	6	1	0
2	F	15	0	7	1	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	7	2	0
3	F	6	0	8	0	0
4	A	223	0	0	1	0
4	B	212	0	0	1	0
4	C	254	0	0	4	0
4	D	186	0	0	1	0
4	E	182	0	0	2	0
4	F	216	0	0	2	0
All	All	15759	0	14165	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (124) 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:D:75:GLU:OE2	4:D:501:HOH:O	1.68	1.10
1:D:63[B]:ARG:HH21	1:D:63[B]:ARG:HG3	1.31	0.91
1:D:63[A]:ARG:HD3	1:F:166:LEU:HD22	1.60	0.83
1:A:166:LEU:HG	1:C:107:PRO:HG2	1.60	0.83
1:E:167[A]:GLU:OE1	4:E:501:HOH:O	2.00	0.79
1:B:166:LEU:HD22	1:E:63:ARG:HD3	1.66	0.78
1:D:166:LEU:HG	1:F:107:PRO:HG2	1.66	0.77
1:B:257[B]:ARG:NH1	4:B:501:HOH:O	2.20	0.74
1:A:167:GLU:OE1	4:A:501:HOH:O	2.07	0.71
1:A:1:MET:HE2	1:A:85:GLY:O	1.90	0.70
1:F:167[A]:GLU:OE1	4:F:501:HOH:O	2.09	0.69
1:A:63[A]:ARG:HD3	1:C:166:LEU:CD2	2.23	0.68
1:A:166:LEU:HD23	1:C:108:ARG:HG3	1.73	0.68
1:C:167:GLU:OE1	4:C:501:HOH:O	2.13	0.67
1:A:63[A]:ARG:HH11	1:C:166:LEU:HD11	1.61	0.66
1:C:63[B]:ARG:HH21	1:C:63[B]:ARG:HG2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286[B]:THR:HG21	1:C:288:ARG:HG3	1.79	0.64
1:D:4:GLU:OE2	1:D:17:SER:HB3	1.97	0.64
1:C:101:LYS:HE2	1:C:109:ASP:OD1	1.99	0.63
1:F:163:LEU:HA	1:F:166:LEU:HD12	1.80	0.62
1:B:7:ILE:HD11	1:B:19:ALA:HB1	1.81	0.62
1:D:63[B]:ARG:HG3	1:D:63[B]:ARG:NH2	2.07	0.62
1:A:63[B]:ARG:HH21	1:A:63[B]:ARG:HG3	1.64	0.61
1:D:82:ARG:HD3	1:D:293:LEU:O	2.01	0.61
1:B:163:LEU:HD23	1:B:166:LEU:HD12	1.81	0.61
1:A:166:LEU:CD2	1:C:108:ARG:HG3	2.31	0.60
1:C:286[B]:THR:HG22	1:C:287:ASP:N	2.16	0.60
1:E:294:SER:OG	1:E:295:GLY:N	2.36	0.59
1:A:63[A]:ARG:NH1	1:C:166:LEU:HD11	2.17	0.59
1:B:158:ARG:NH2	2:B:401:PLP:O3	2.30	0.58
1:D:101:LYS:NZ	1:D:109:ASP:OD1	2.36	0.58
1:A:63[A]:ARG:HD3	1:C:166:LEU:HD21	1.85	0.58
1:B:7:ILE:HD11	1:B:19:ALA:CB	2.34	0.58
1:A:1:MET:N	1:A:84:ASN:O	2.26	0.58
1:B:165:ARG:HH21	1:B:165:ARG:HG3	1.69	0.57
1:C:63[B]:ARG:HH21	1:C:63[B]:ARG:CG	2.17	0.57
1:B:82[A]:ARG:HH11	1:B:297:HIS:CE1	2.23	0.57
1:B:107:PRO:HG2	1:E:166:LEU:HG	1.87	0.56
1:D:107:PRO:HG2	1:F:166:LEU:HG	1.88	0.56
1:D:166:LEU:HD23	1:F:108:ARG:HG3	1.88	0.55
1:A:63[B]:ARG:HG3	1:A:63[B]:ARG:NH2	2.21	0.54
1:E:126:ASP:O	1:E:130[B]:ARG:HG3	2.06	0.54
1:A:63[A]:ARG:HD3	1:C:166:LEU:CD1	2.37	0.54
1:F:185:VAL:HG11	1:F:193:LEU:HD22	1.90	0.54
1:F:210[B]:ARG:NH1	4:F:505:HOH:O	2.40	0.54
1:B:163:LEU:HD23	1:B:166:LEU:CD1	2.37	0.54
1:D:3:ASP:N	1:D:3:ASP:OD1	2.41	0.54
1:A:2:SER:OG	1:A:3:ASP:N	2.41	0.53
1:B:163:LEU:HA	1:B:166:LEU:HD12	1.90	0.53
1:C:286[B]:THR:CG2	1:C:288:ARG:HG3	2.38	0.53
1:B:166:LEU:HG	1:E:107:PRO:HG2	1.91	0.52
1:E:161:SER:HB2	1:E:189:ALA:HB2	1.91	0.52
1:A:63[B]:ARG:NH2	1:F:261:GLY:O	2.43	0.51
1:B:282:ALA:O	1:B:286:THR:HG23	2.11	0.51
1:E:154:LYS:NZ	2:E:401:PLP:O3	2.44	0.50
1:C:77:ILE:HG23	1:C:91:ILE:HG21	1.94	0.50
1:A:63[A]:ARG:CD	1:C:166:LEU:HD21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:HG11	1:B:193:LEU:HD22	1.94	0.50
1:B:70[B]:ARG:HG2	1:B:70[B]:ARG:HH21	1.77	0.49
1:F:154:LYS:NZ	2:F:401:PLP:O3	2.43	0.49
1:E:4:GLU:OE2	1:E:17:SER:HB3	2.12	0.49
1:F:185:VAL:HG11	1:F:193:LEU:CD2	2.43	0.48
1:C:79:GLU:O	1:C:83:ARG:HG2	2.14	0.48
1:A:166:LEU:HD11	1:C:107:PRO:HB2	1.96	0.48
1:B:185:VAL:HG11	1:B:193:LEU:CD2	2.44	0.48
1:A:213:THR:O	1:A:217:ILE:HG12	2.14	0.48
1:B:126:ASP:O	1:B:130:ARG:HG3	2.14	0.47
1:C:71:ASP:O	1:C:75[A]:GLU:HG2	2.15	0.47
1:E:4:GLU:OE2	1:E:17:SER:CB	2.62	0.47
1:B:48:LEU:HD21	1:B:74:LYS:HG3	1.97	0.47
1:E:163:LEU:HD23	1:E:166:LEU:HD12	1.96	0.47
1:C:63[B]:ARG:HG2	1:C:63[B]:ARG:NH2	2.26	0.47
1:A:161:SER:HB2	1:A:189:ALA:HB2	1.96	0.46
1:D:126:ASP:OD1	1:D:129:LYS:HG2	2.14	0.46
1:C:210[B]:ARG:HG2	1:C:210[B]:ARG:HH21	1.80	0.46
1:C:210[B]:ARG:NH1	4:C:505:HOH:O	2.48	0.46
1:D:161:SER:HB2	1:D:189:ALA:HB2	1.97	0.46
3:E:402:GOL:H2	4:E:572:HOH:O	2.16	0.45
1:D:154:LYS:NZ	2:D:401:PLP:O3	2.48	0.45
1:A:63[B]:ARG:HH21	1:A:63[B]:ARG:CG	2.30	0.45
1:B:108:ARG:HG3	1:E:166:LEU:HD23	1.98	0.45
1:F:163:LEU:HD23	1:F:166:LEU:HD12	1.99	0.44
1:C:231[A]:ARG:HG2	1:C:232:GLN:O	2.17	0.44
1:B:66:HIS:HB2	1:B:112:PRO:HG3	1.99	0.44
1:B:70[B]:ARG:HG2	1:B:70[B]:ARG:NH2	2.33	0.44
1:B:77:ILE:HG23	1:B:91:ILE:HG21	1.99	0.44
1:A:1:MET:CE	1:A:85:GLY:O	2.64	0.44
1:A:167:GLU:CD	1:B:262:ARG:HH22	2.21	0.44
1:F:213:THR:O	1:F:217:ILE:HG12	2.18	0.44
1:B:213:THR:O	1:B:217:ILE:HG12	2.18	0.44
1:D:282:ALA:O	1:D:286:THR:HG23	2.18	0.43
1:A:185:VAL:HG11	1:A:193:LEU:HD22	2.00	0.43
1:C:185:VAL:HG11	1:C:193:LEU:HD22	2.00	0.43
1:D:166:LEU:HG	1:F:107:PRO:CG	2.40	0.43
1:C:213:THR:O	1:C:217:ILE:HG12	2.19	0.43
1:A:63[A]:ARG:HD3	1:C:166:LEU:HD11	2.00	0.43
1:D:65:ASN:HD22	1:D:65:ASN:H	1.67	0.43
1:D:213:THR:O	1:D:217:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASN:H	1:D:65:ASN:ND2	2.18	0.42
1:C:154:LYS:NZ	2:C:401:PLP:O3	2.52	0.42
1:F:8:TYR:O	1:F:115:ILE:HA	2.20	0.42
1:E:185:VAL:HG11	1:E:193:LEU:HD22	2.02	0.42
1:C:48:LEU:HD21	1:C:74:LYS:HG3	2.00	0.42
1:D:125:ALA:HB1	1:D:129:LYS:HB2	2.02	0.42
1:B:161:SER:HB2	1:B:189:ALA:HB2	2.02	0.42
1:C:286[B]:THR:HG22	1:C:288:ARG:H	1.83	0.41
1:E:66:HIS:HB2	1:E:112:PRO:HG3	2.01	0.41
1:E:100:PRO:HB2	1:E:102:GLY:O	2.20	0.41
1:B:24:VAL:HA	1:B:29:LEU:HD11	2.02	0.41
1:C:161:SER:HB2	1:C:189:ALA:HB2	2.02	0.41
1:A:48:LEU:HD21	1:A:74:LYS:HG3	2.02	0.41
1:C:127[B]:GLU:HG3	4:C:717:HOH:O	2.21	0.41
3:E:402:GOL:HO1	1:F:210[B]:ARG:HH11	1.68	0.41
1:E:127:GLU:OE2	1:E:130[B]:ARG:NH1	2.54	0.41
1:E:77:ILE:HG23	1:E:91:ILE:HG21	2.03	0.41
1:F:163:LEU:HD23	1:F:166:LEU:CD1	2.50	0.41
1:A:154:LYS:NZ	2:A:401:PLP:O3	2.54	0.40
1:F:77:ILE:HG23	1:F:91:ILE:HG21	2.03	0.40
1:C:231[B]:ARG:NH1	4:C:512:HOH:O	2.54	0.40
1:A:126:ASP:O	1:A:130[A]:ARG:HG3	2.21	0.40
1:B:82[A]:ARG:NH1	1:B:297:HIS:CE1	2.88	0.40
1:A:97:ARG:HD2	1:A:107:PRO:HA	2.03	0.40
1:D:77:ILE:HG23	1:D:91:ILE:HG21	2.04	0.40
1:D:201:LEU:O	1:D:228:TRP:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	297/302 (98%)	292 (98%)	5 (2%)	0	100 100
1	B	304/302 (101%)	300 (99%)	4 (1%)	0	100 100
1	C	304/302 (101%)	298 (98%)	6 (2%)	0	100 100
1	D	299/302 (99%)	294 (98%)	4 (1%)	1 (0%)	41 21
1	E	300/302 (99%)	293 (98%)	7 (2%)	0	100 100
1	F	298/302 (99%)	293 (98%)	5 (2%)	0	100 100
All	All	1802/1812 (99%)	1770 (98%)	31 (2%)	1 (0%)	51 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	GLY

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	249/252 (99%)	247 (99%)	2 (1%)	81 70
1	B	256/252 (102%)	253 (99%)	3 (1%)	71 54
1	C	256/252 (102%)	252 (98%)	4 (2%)	62 41
1	D	251/252 (100%)	247 (98%)	4 (2%)	62 41
1	E	252/252 (100%)	249 (99%)	3 (1%)	71 54
1	F	250/252 (99%)	248 (99%)	2 (1%)	81 70
All	All	1514/1512 (100%)	1496 (99%)	18 (1%)	76 54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ASP
1	A	165	ARG
1	B	70[A]	ARG
1	B	70[B]	ARG

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Mol	Chain	Res	Type
1	B	157	ASP
1	C	97	ARG
1	C	157	ASP
1	C	175[A]	ASP
1	C	175[B]	ASP
1	D	157	ASP
1	D	175	ASP
1	D	231[A]	ARG
1	D	231[B]	ARG
1	E	157	ASP
1	E	231[A]	ARG
1	E	231[B]	ARG
1	F	157	ASP
1	F	231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	18	GLN
1	D	65	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

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

12 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

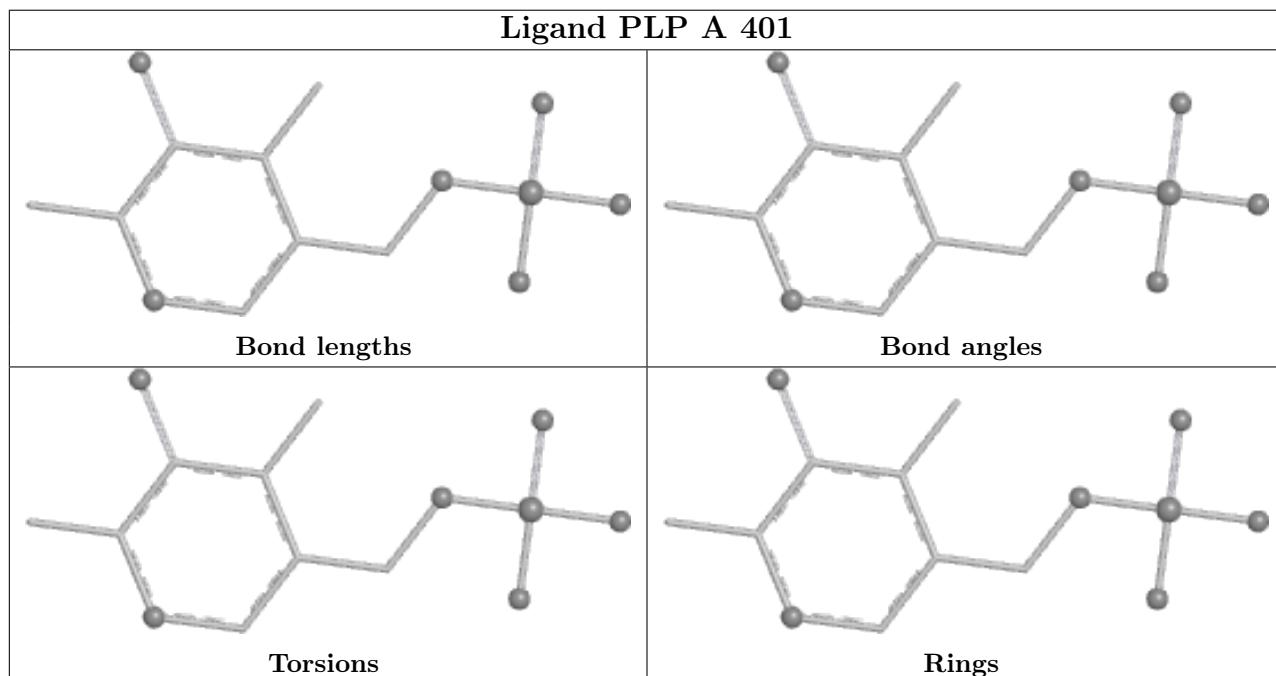
There are no chirality outliers.

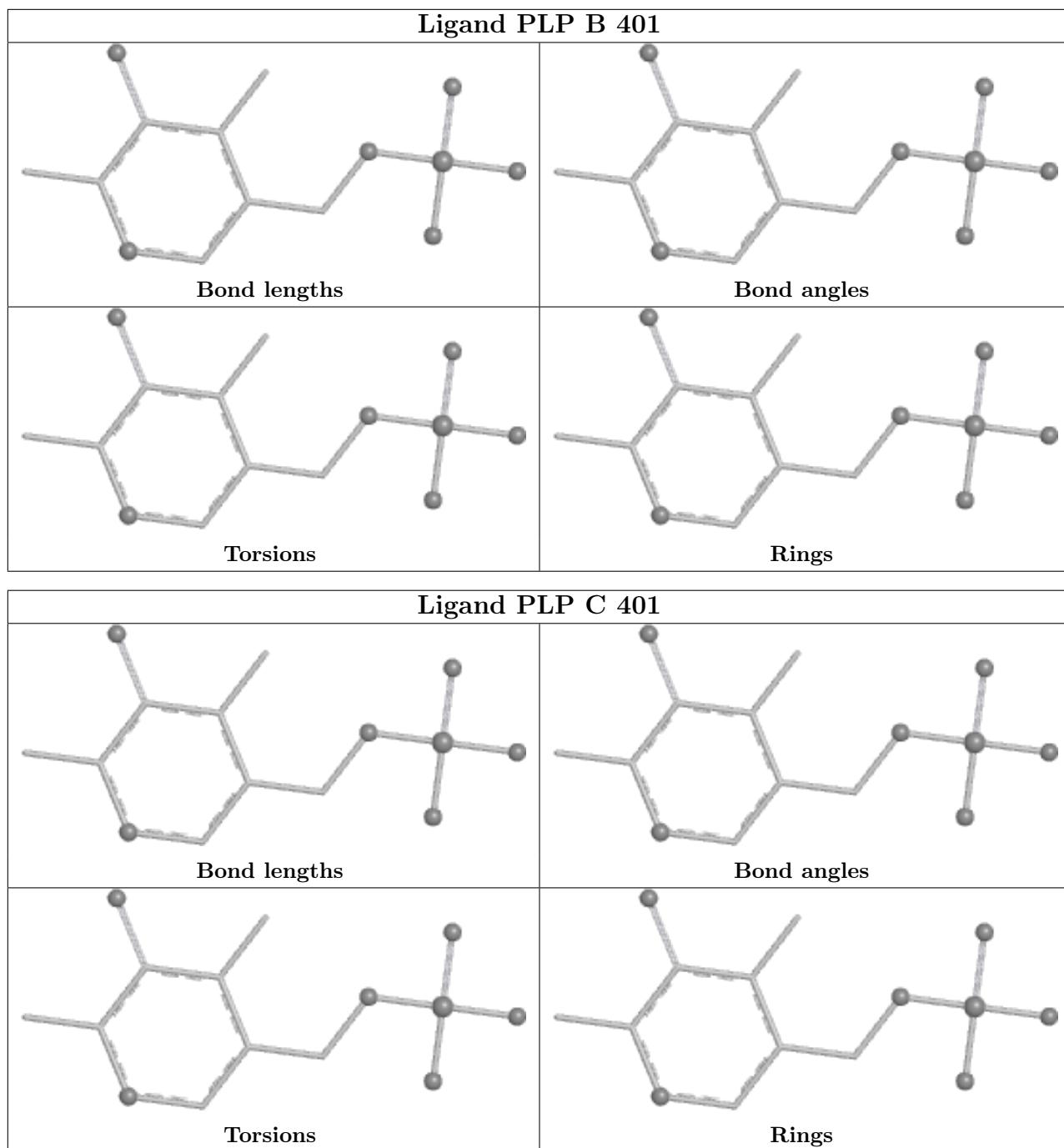
There are no torsion outliers.

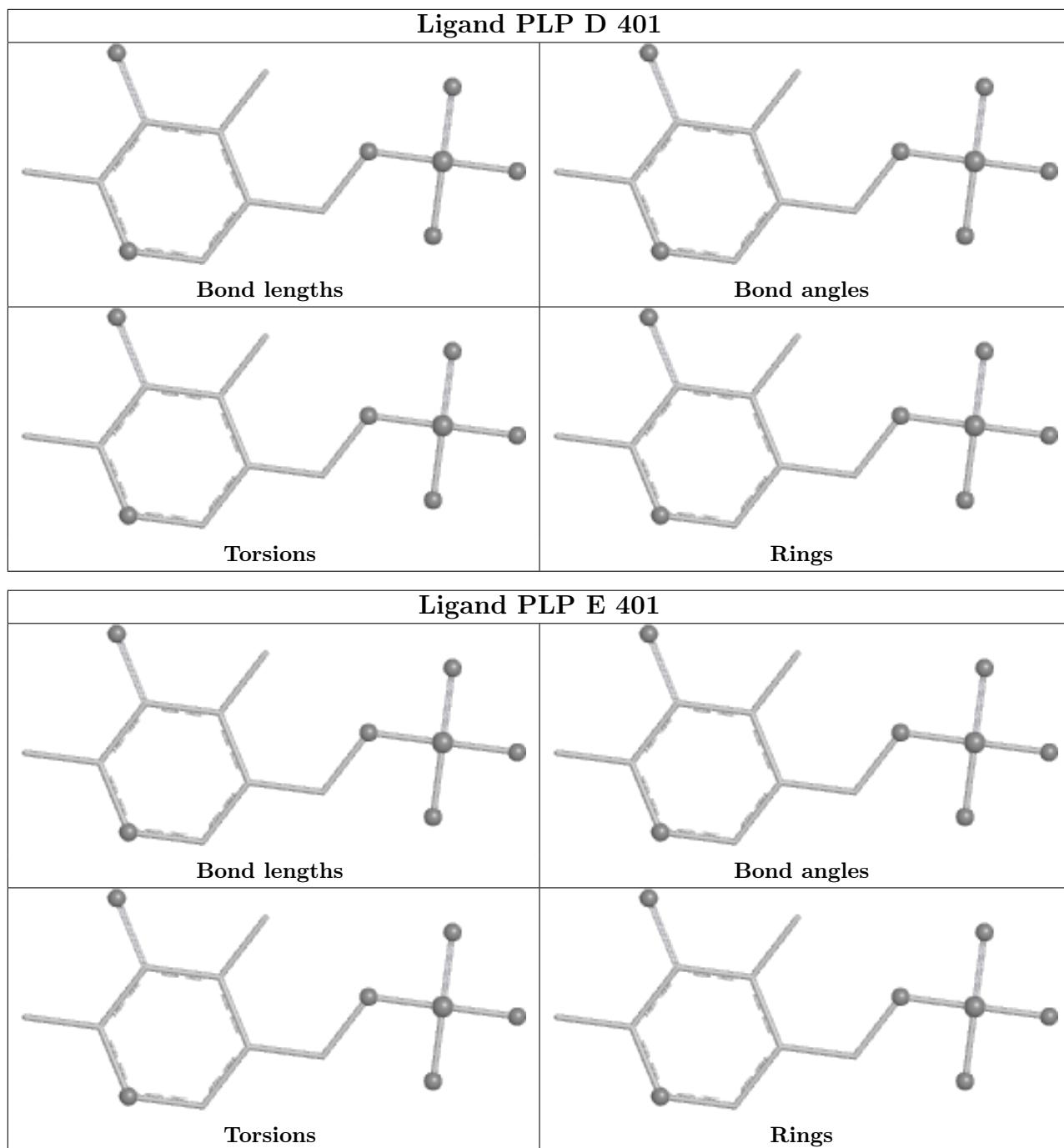
There are no ring outliers.

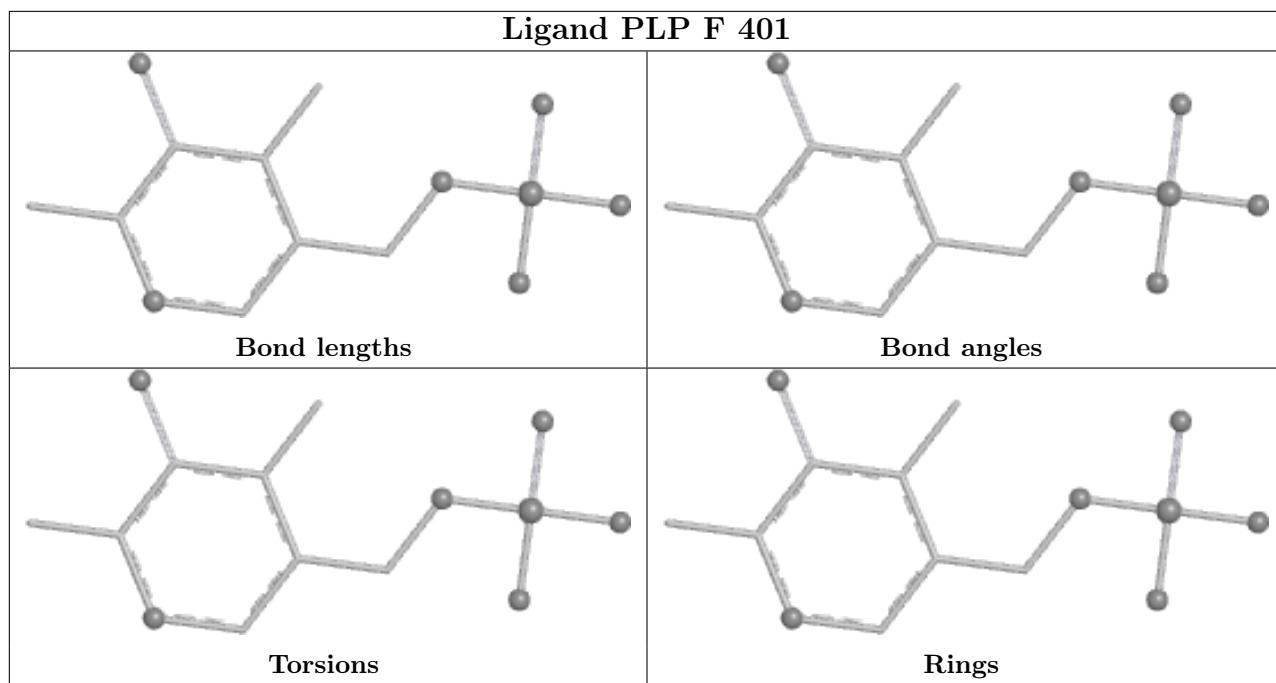
No monomer is involved in short contacts.

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









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 (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	296/302 (98%)	1.22	48 (16%) 1 1	20, 28, 50, 73	0
1	B	299/302 (99%)	1.46	71 (23%) 0 0	20, 30, 53, 79	0
1	C	294/302 (97%)	1.15	32 (10%) 5 4	20, 27, 43, 84	0
1	D	295/302 (97%)	1.35	57 (19%) 1 1	21, 32, 55, 101	0
1	E	294/302 (97%)	1.25	44 (14%) 2 1	21, 32, 55, 80	0
1	F	294/302 (97%)	1.31	44 (14%) 2 1	20, 29, 51, 84	0
All	All	1772/1812 (97%)	1.29	296 (16%) 1 1	20, 30, 52, 101	0

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	103	VAL	18.5
1	F	2	SER	15.0
1	C	2	SER	14.9
1	B	103	VAL	13.6
1	F	103	VAL	13.2
1	F	104	VAL	12.2
1	D	2	SER	11.8
1	D	103	VAL	10.8
1	E	2	SER	10.7
1	A	1	MET	10.2
1	D	3	ASP	9.7
1	B	102	GLY	9.6
1	A	103	VAL	9.3
1	D	295	GLY	9.1
1	C	102	GLY	8.5
1	B	3	ASP	8.3
1	F	3	ASP	8.3
1	B	104	VAL	8.3
1	A	102	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLY	8.1
1	E	295	GLY	7.7
1	E	3	ASP	7.7
1	F	105	ALA	7.5
1	C	105	ALA	7.4
1	F	100	PRO	7.3
1	A	104	VAL	7.2
1	F	102	GLY	7.1
1	B	2	SER	7.0
1	E	103	VAL	6.8
1	C	104	VAL	6.5
1	B	287	ASP	6.4
1	B	105	ALA	6.4
1	A	296	SER	6.2
1	D	287	ASP	5.9
1	E	286	THR	5.9
1	A	295	GLY	5.8
1	A	2	SER	5.7
1	B	286	THR	5.7
1	C	3	ASP	5.6
1	E	104	VAL	5.5
1	E	181[A]	HIS	5.4
1	B	181[A]	HIS	5.4
1	E	102	GLY	5.3
1	E	287	ASP	5.3
1	A	100	PRO	5.2
1	D	296	SER	5.1
1	E	294	SER	5.1
1	B	296	SER	5.0
1	E	122	ILE	5.0
1	B	300	HIS	5.0
1	D	104	VAL	4.8
1	F	294	SER	4.8
1	C	286[A]	THR	4.7
1	B	299	HIS	4.7
1	B	295	GLY	4.7
1	B	16	LEU	4.6
1	A	282	ALA	4.3
1	C	287	ASP	4.2
1	A	105	ALA	4.1
1	C	225	ASP	4.1
1	E	293	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	266	GLY	3.9
1	A	287	ASP	3.9
1	E	100	PRO	3.8
1	E	13	TYR	3.8
1	A	3	ASP	3.8
1	D	225	ASP	3.8
1	B	298	HIS	3.7
1	D	15	PRO	3.7
1	B	297	HIS	3.7
1	D	86	LEU	3.7
1	A	225	ASP	3.6
1	F	7	ILE	3.6
1	D	294	SER	3.6
1	B	109	ASP	3.5
1	B	225	ASP	3.5
1	B	267	THR	3.4
1	C	100	PRO	3.4
1	D	14	LEU	3.4
1	A	164	ILE	3.4
1	F	179	LEU	3.4
1	C	179	LEU	3.3
1	E	86	LEU	3.3
1	F	149	LEU	3.3
1	B	281	TRP	3.3
1	D	149	LEU	3.3
1	F	166	LEU	3.3
1	C	101	LYS	3.3
1	B	179	LEU	3.2
1	C	182[A]	SER	3.2
1	F	67	ASP	3.2
1	F	13	TYR	3.2
1	E	120	PRO	3.2
1	F	86	LEU	3.1
1	B	138	ILE	3.1
1	F	164	ILE	3.1
1	D	222	THR	3.1
1	E	282	ALA	3.1
1	A	222	THR	3.1
1	A	288	ARG	3.1
1	B	285	GLU	3.1
1	C	107	PRO	3.1
1	C	127[A]	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	16	LEU	3.1
1	A	131	ARG	3.0
1	D	100	PRO	3.0
1	A	179	LEU	3.0
1	D	281	TRP	3.0
1	F	293	LEU	3.0
1	B	144	PHE	3.0
1	E	288	ARG	2.9
1	F	225	ASP	2.9
1	E	14	LEU	2.9
1	D	75	GLU	2.9
1	B	159	LEU	2.9
1	B	100	PRO	2.9
1	F	106	ASP	2.9
1	A	267	THR	2.9
1	C	166	LEU	2.9
1	A	272	ILE	2.9
1	E	149	LEU	2.8
1	E	67	ASP	2.8
1	A	285	GLU	2.8
1	D	18	GLN	2.8
1	E	131[A]	ARG	2.8
1	F	177	LEU	2.8
1	E	42	LYS	2.8
1	D	148	THR	2.8
1	B	101	LYS	2.8
1	C	224	LEU	2.8
1	E	71	ASP	2.8
1	D	278	ASN	2.8
1	F	101	LYS	2.8
1	A	289	TYR	2.7
1	C	109	ASP	2.7
1	F	159	LEU	2.7
1	C	146	ALA	2.7
1	D	105	ALA	2.7
1	F	178	TRP	2.7
1	B	153[A]	TYR	2.7
1	D	64	LEU	2.7
1	D	179	LEU	2.7
1	D	182	SER	2.7
1	B	70[A]	ARG	2.7
1	D	81	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	271	PRO	2.7
1	D	146	ALA	2.6
1	C	295	GLY	2.6
1	B	208	ILE	2.6
1	D	67	ASP	2.6
1	B	206	ALA	2.6
1	B	131	ARG	2.6
1	D	291	THR	2.6
1	F	109	ASP	2.6
1	B	226	ILE	2.6
1	D	127[A]	GLU	2.6
1	C	149	LEU	2.6
1	D	273	THR	2.6
1	E	34	VAL	2.6
1	D	153[A]	TYR	2.6
1	F	153[A]	TYR	2.6
1	F	222	THR	2.5
1	D	144	PHE	2.5
1	E	290	ALA	2.5
1	D	268	THR	2.5
1	D	122	ILE	2.5
1	D	289	TYR	2.5
1	E	267	THR	2.5
1	A	226	ILE	2.5
1	C	208	ILE	2.5
1	D	21	VAL	2.5
1	A	159	LEU	2.5
1	A	126	ASP	2.5
1	A	127	GLU	2.5
1	E	101	LYS	2.5
1	F	5	PRO	2.5
1	C	138	ILE	2.5
1	E	77	ILE	2.5
1	E	78	ILE	2.5
1	A	148	THR	2.4
1	F	18[A]	GLN	2.4
1	B	185	VAL	2.4
1	B	217	ILE	2.4
1	F	14	LEU	2.4
1	A	4	GLU	2.4
1	A	223	GLU	2.4
1	A	153[A]	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	294	SER	2.4
1	A	122	ILE	2.4
1	B	52	LEU	2.4
1	B	235	ALA	2.4
1	A	140	ALA	2.4
1	A	217	ILE	2.4
1	B	48	LEU	2.4
1	B	156	LEU	2.4
1	B	276	ILE	2.4
1	D	286	THR	2.4
1	B	118	VAL	2.3
1	E	210[A]	ARG	2.3
1	A	163	LEU	2.3
1	B	155	CYS	2.3
1	E	225	ASP	2.3
1	C	153[A]	TYR	2.3
1	B	146	ALA	2.3
1	E	146	ALA	2.3
1	B	140	ALA	2.3
1	F	146	ALA	2.3
1	B	223	GLU	2.3
1	D	120	PRO	2.3
1	B	182[A]	SER	2.3
1	B	209	LEU	2.3
1	D	293	LEU	2.3
1	B	164	ILE	2.3
1	E	126	ASP	2.3
1	A	144	PHE	2.3
1	B	282	ALA	2.3
1	C	140	ALA	2.3
1	F	127	GLU	2.3
1	A	238	VAL	2.3
1	D	226	ILE	2.3
1	F	114	CYS	2.3
1	F	144	PHE	2.3
1	B	17	SER	2.2
1	A	149	LEU	2.2
1	B	86	LEU	2.2
1	D	220	LEU	2.2
1	A	270	GLY	2.2
1	E	128	GLU	2.2
1	B	13	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	34	VAL	2.2
1	E	64	LEU	2.2
1	B	7	ILE	2.2
1	F	69[A]	SER	2.2
1	B	145	PRO	2.2
1	B	151	PRO	2.2
1	C	219[A]	GLU	2.2
1	C	222	THR	2.2
1	B	177	LEU	2.2
1	D	4	GLU	2.2
1	D	71	ASP	2.2
1	B	294	SER	2.2
1	A	208	ILE	2.2
1	F	59	ILE	2.2
1	F	264	ILE	2.2
1	F	145	PRO	2.2
1	B	270	GLY	2.2
1	C	148	THR	2.2
1	A	283	MET	2.2
1	E	116	VAL	2.2
1	B	136	LEU	2.2
1	B	274	GLN	2.2
1	F	209	LEU	2.2
1	D	9	ILE	2.2
1	D	285	GLU	2.2
1	F	167[A]	GLU	2.2
1	F	208	ILE	2.2
1	B	178	TRP	2.2
1	D	178	TRP	2.2
1	D	8	TYR	2.1
1	E	123	PHE	2.1
1	F	136	LEU	2.1
1	E	148	THR	2.1
1	B	228	TRP	2.1
1	E	41	TRP	2.1
1	B	18	GLN	2.1
1	F	38	VAL	2.1
1	C	267	THR	2.1
1	D	177	LEU	2.1
1	E	4	GLU	2.1
1	A	146	ALA	2.1
1	B	149	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	63[A]	ARG	2.1
1	A	269	PRO	2.1
1	F	120	PRO	2.1
1	B	85	GLY	2.1
1	D	208	ILE	2.1
1	C	185	VAL	2.1
1	B	293	LEU	2.1
1	D	218	LEU	2.1
1	D	165	ARG	2.0
1	B	141	THR	2.0
1	D	250	ALA	2.0
1	B	238	VAL	2.0
1	E	233	LEU	2.0
1	F	156	LEU	2.0
1	A	141	THR	2.0
1	C	247	CYS	2.0
1	E	81	THR	2.0
1	D	62	ALA	2.0
1	B	288	ARG	2.0
1	D	288	ARG	2.0
1	B	4	GLU	2.0
1	C	285	GLU	2.0
1	A	166	LEU	2.0
1	A	183	GLY	2.0
1	B	292	PRO	2.0

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 [\(i\)](#)

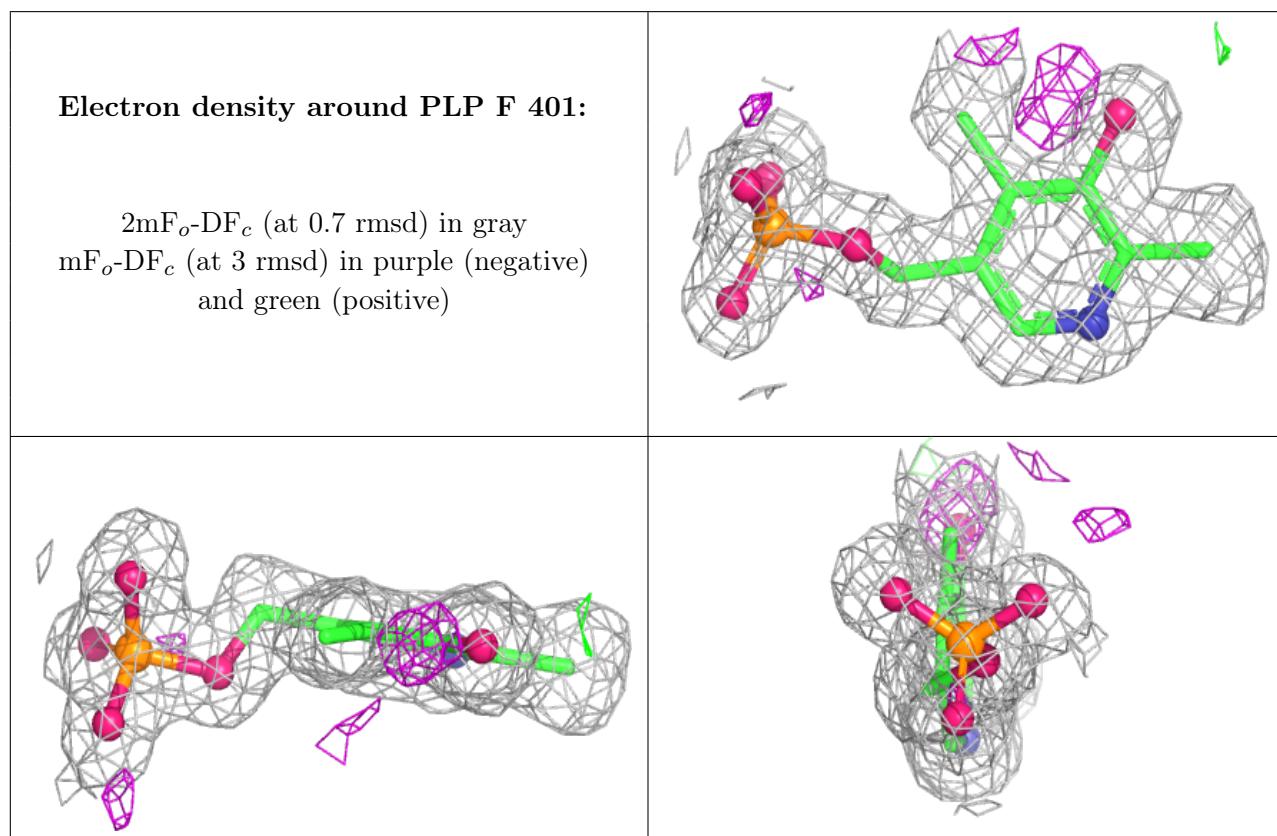
There are no monosaccharides in this entry.

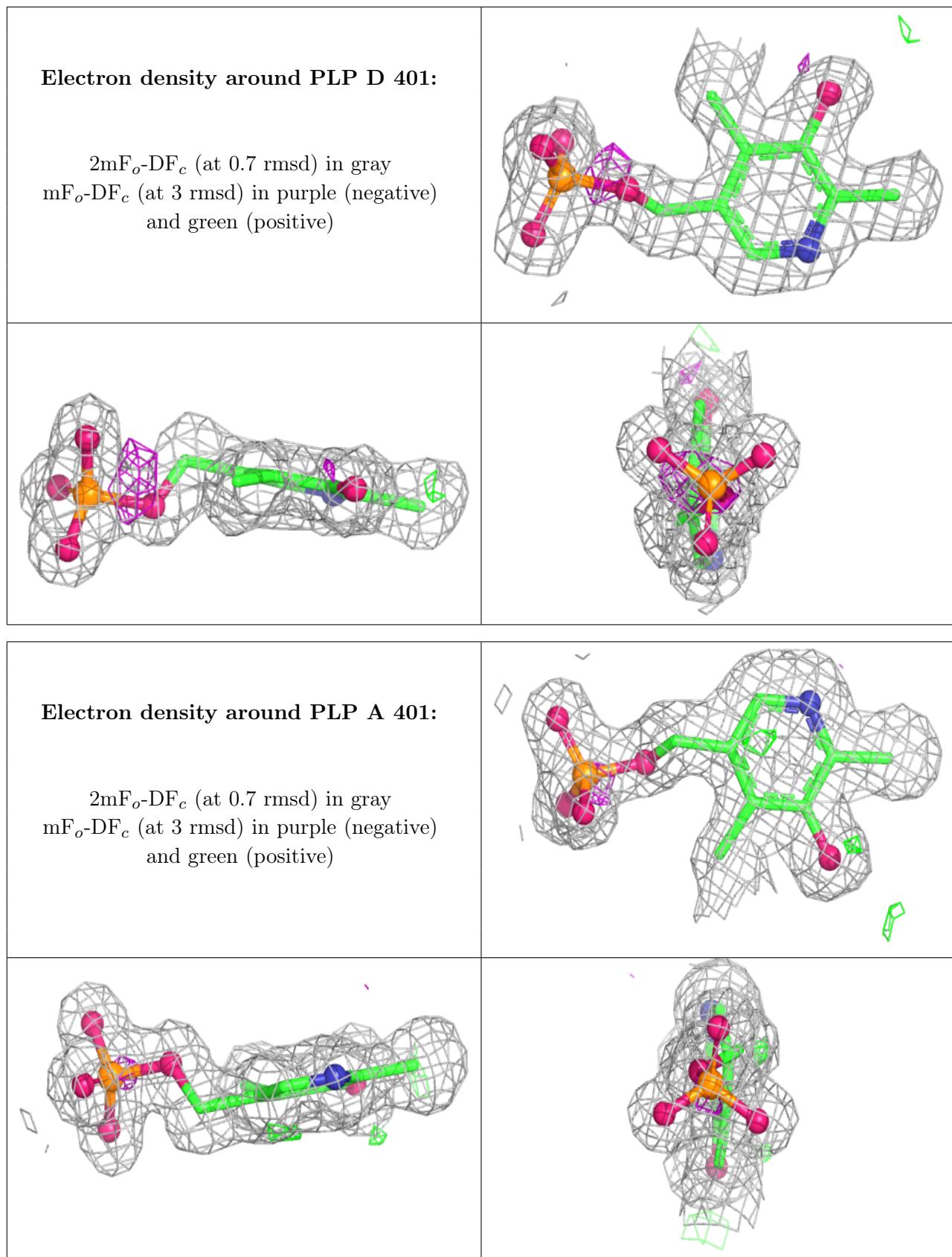
6.4 Ligands [\(i\)](#)

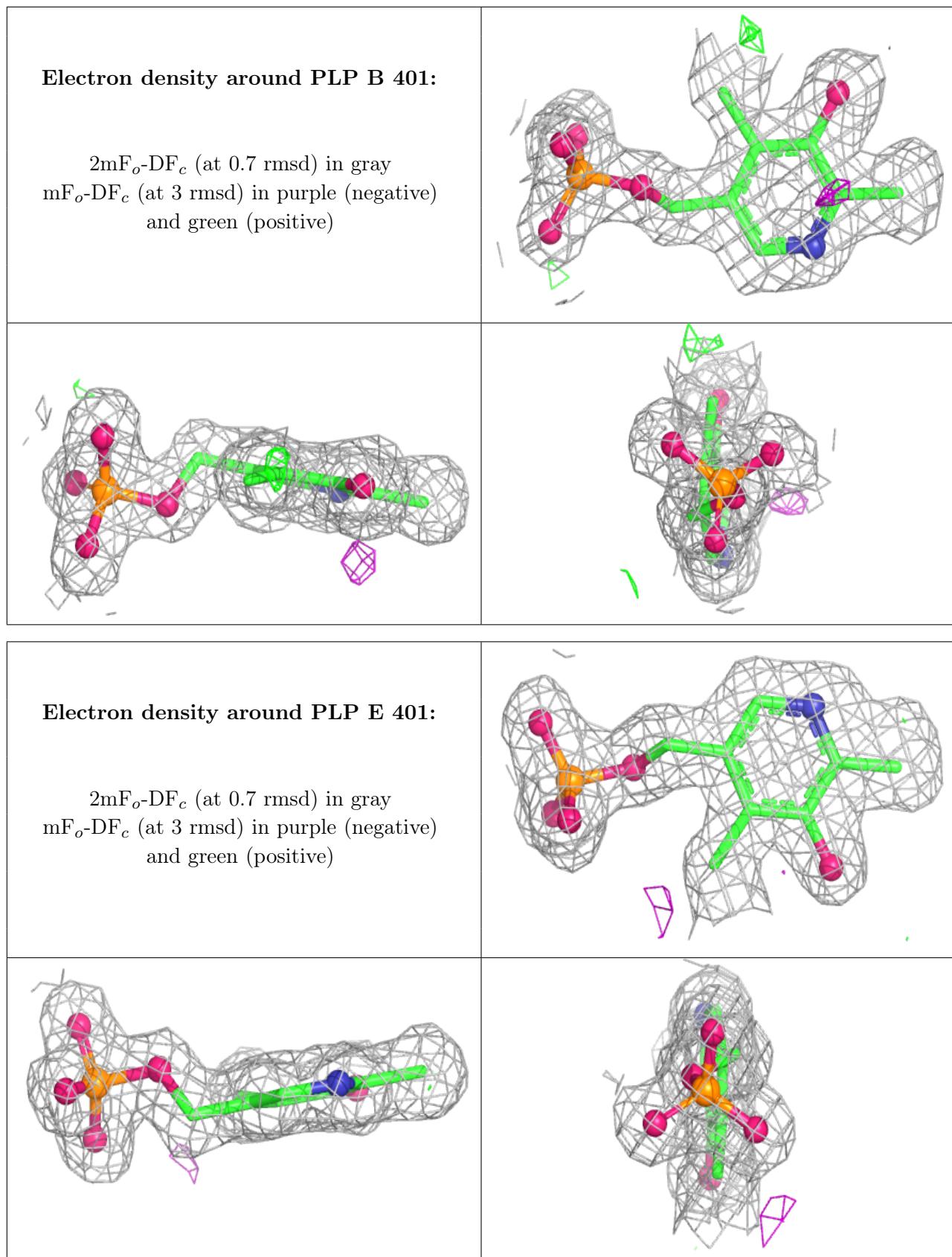
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

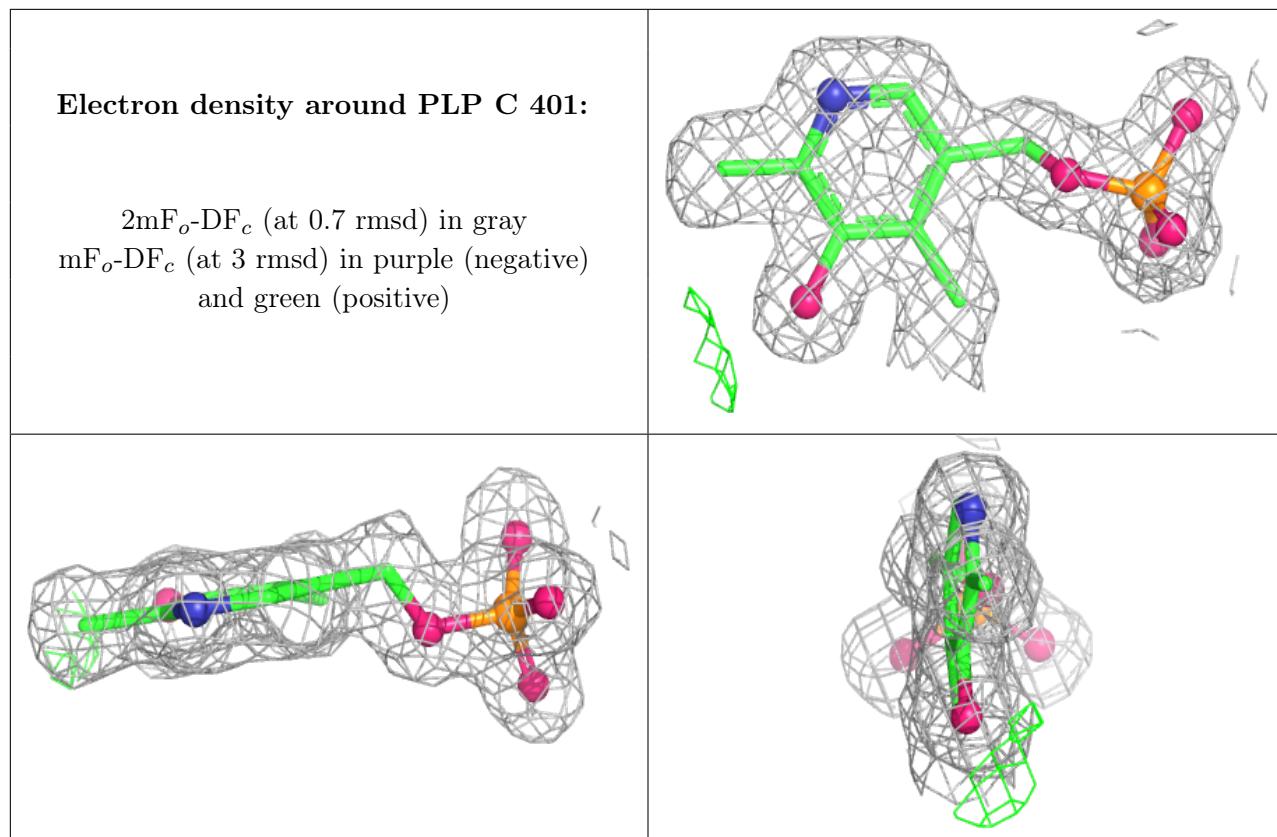
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	E	402	6/6	0.70	0.19	49,58,66,67	0
3	GOL	D	402	6/6	0.75	0.14	40,44,49,50	0
3	GOL	C	402	6/6	0.79	0.15	43,48,53,54	0
3	GOL	F	402	6/6	0.80	0.11	38,39,42,43	0
3	GOL	B	402	6/6	0.81	0.16	34,35,36,37	0
3	GOL	A	402	6/6	0.83	0.16	44,52,61,62	0
2	PLP	F	401	15/16	0.89	0.13	22,24,25,25	0
2	PLP	D	401	15/16	0.90	0.13	25,26,27,27	0
2	PLP	A	401	15/16	0.90	0.12	21,23,25,26	0
2	PLP	B	401	15/16	0.91	0.13	23,24,25,26	0
2	PLP	E	401	15/16	0.93	0.10	23,25,26,27	0
2	PLP	C	401	15/16	0.94	0.10	19,22,23,26	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.









6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.