



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 12:24 PM EDT

PDB ID : 8E0Y
Title : DAHP (3-deoxy-D-arabinoheptulosonate-7-phosphate) Synthase complexed with DAHP oxime, Pr(III), and Pi in unbound:(bound)2:other Conformations
Authors : Berti, P.J.; Junop, M.S.; Grainger, R.
Deposited on : 2022-08-09
Resolution : 2.01 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

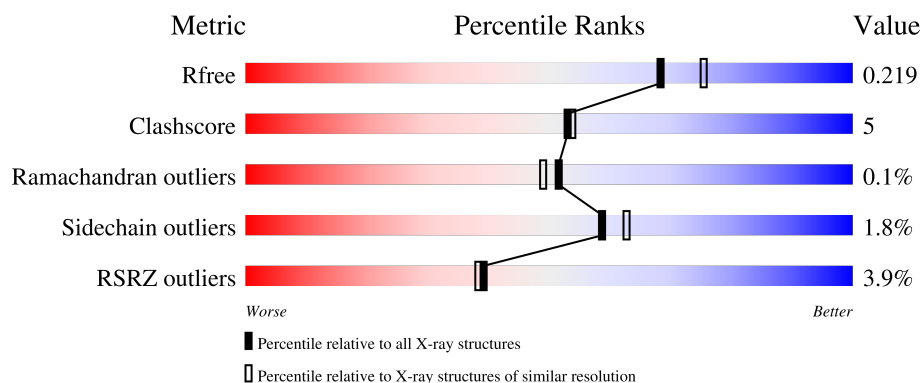
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	351	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>••</div> </div>
1	B	351	<div> <div>4%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
1	C	351	<div> <div>89%</div> <div>9%</div> <div>•</div> </div>
1	D	351	<div> <div>8%</div> <div>80%</div> <div>16%</div> <div>•</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10915 atoms, of which 23 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 Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	1	0
			2551	1602	453	481	15			
1	B	340	Total	C	N	O	S	0	0	0
			2523	1586	449	474	14			
1	C	344	Total	C	N	O	S	0	0	0
			2587	1624	460	489	14			
1	D	336	Total	C	N	O	S	0	1	0
			2498	1566	444	473	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P0AB91
B	0	GLY	-	expression tag	UNP P0AB91
C	0	GLY	-	expression tag	UNP P0AB91
D	0	GLY	-	expression tag	UNP P0AB91

- Molecule 2 is PRASEODYMIUM ION (three-letter code: PR) (formula: Pr) (labeled as "Ligand of Interest" by depositor).

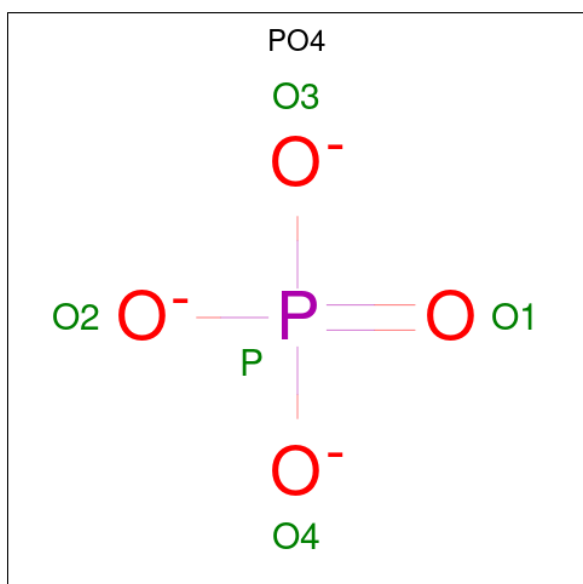
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Pr	0	0
			2	2		
2	B	2	Total	Pr	0	0
			2	2		
2	C	2	Total	Pr	0	0
			2	2		
2	D	2	Total	Pr	0	0
			2	2		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			18	6	5	7		
3	B	1	Total	C	H	O	0	0
			18	6	5	7		
3	C	1	Total	C	H	O	0	0
			18	6	5	7		
3	D	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



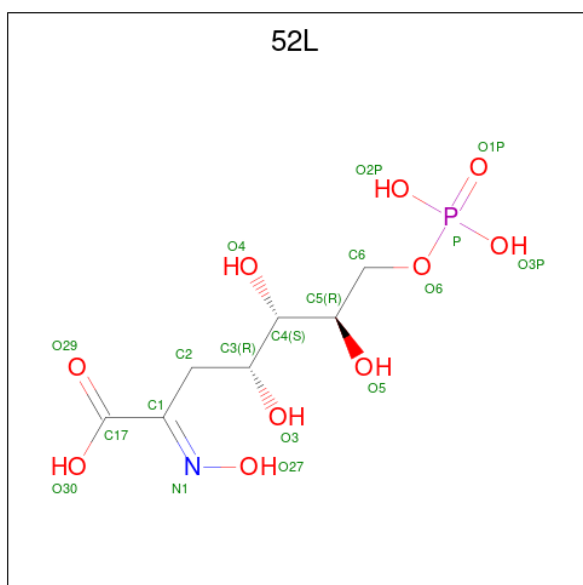
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 6 is DAHP Oxime (three-letter code: 52L) (formula: $C_7H_{14}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			19	7	1	10	1		

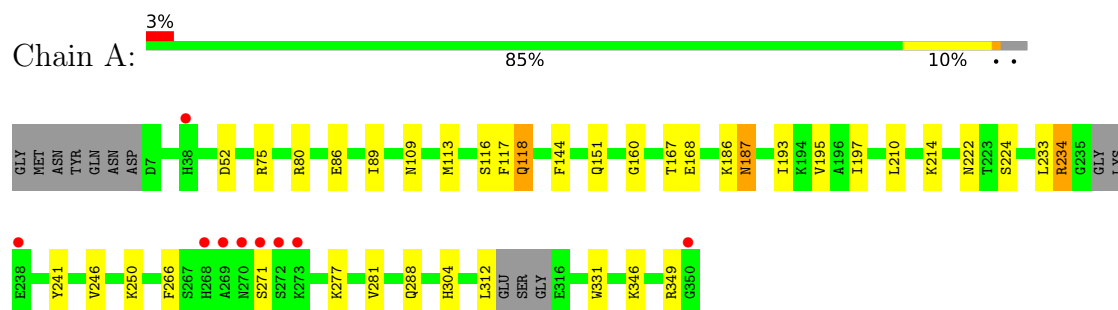
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	179	Total	O	0	0
			179	179		
7	B	80	Total	O	0	0
			80	80		
7	C	280	Total	O	0	0
			280	280		
7	D	106	Total	O	0	0
			106	106		

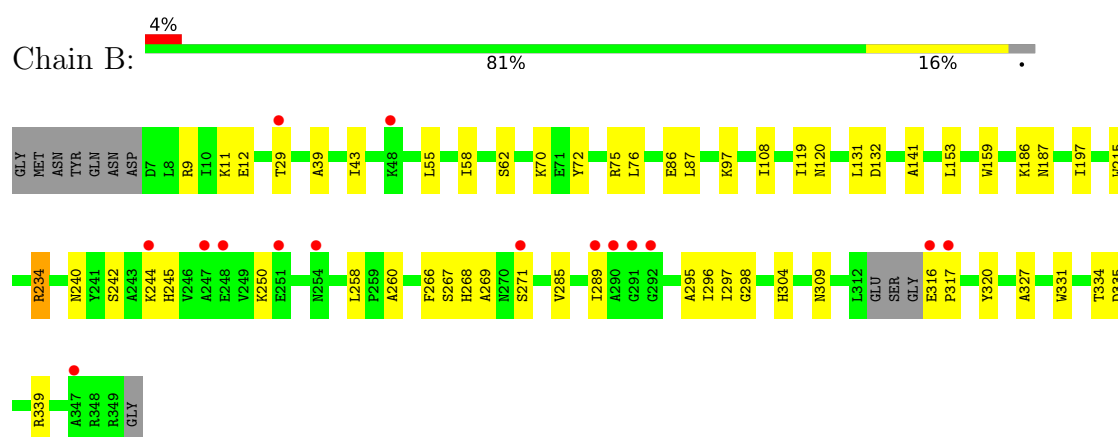
3 Residue-property plots [i](#)

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.

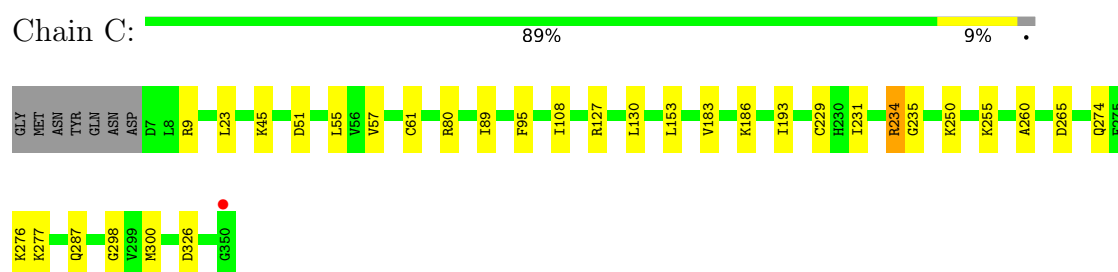
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive



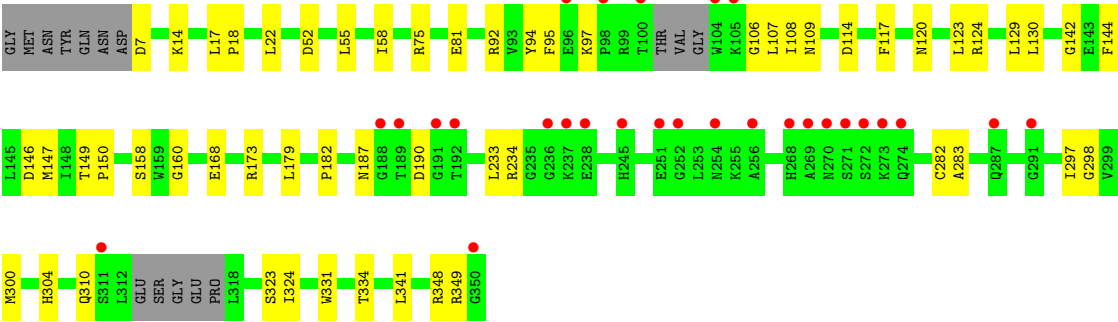
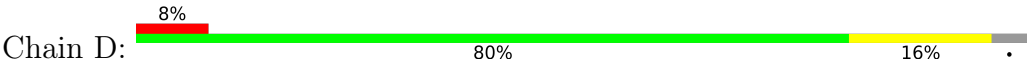
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive



- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, Phe-sensitive



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.85Å 53.25Å 150.54Å 90.00° 115.59° 90.00°	Depositor
Resolution (Å)	46.47 – 2.01 46.47 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.47-2.01) 97.4 (46.47-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.202 , 0.219 0.201 , 0.219	Depositor DCC
R_{free} test set	4906 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10915	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 3.97% 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: FLC, PR, PO4, 52L, ACT

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	0.48	0/2594	0.67	0/3514
1	B	0.50	0/2567	0.66	0/3487
1	C	0.50	0/2632	0.66	0/3566
1	D	0.56	0/2543	0.70	0/3453
All	All	0.51	0/10336	0.67	0/14020

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	2551	0	2523	27	0
1	B	2523	0	2478	35	0
1	C	2587	0	2577	17	0
1	D	2498	0	2433	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	13	5	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	5	5	2	0
3	C	13	5	5	0	0
3	D	13	5	5	1	0
4	B	5	0	0	0	0
5	B	4	3	3	0	0
6	C	19	0	0	0	0
7	A	179	0	0	0	0
7	B	80	0	0	2	0
7	C	280	0	0	1	0
7	D	106	0	0	3	0
All	All	10892	23	10034	109	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 5.

All (109) 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:250:LYS:HG2	1:B:260:ALA:HB1	1.50	0.90
1:D:120:ASN:HB2	3:D:403:FLC:HG2	1.72	0.70
1:B:58:ILE:HD11	1:B:334:THR:HG23	1.79	0.64
1:B:250:LYS:HD3	1:B:295:ALA:HB2	1.78	0.64
1:A:113:MET:HB3	1:A:312:LEU:HD21	1.83	0.60
1:B:120:ASN:HB2	3:B:404:FLC:HG2	1.83	0.60
1:C:45:LYS:HG2	1:C:51:ASP:HB2	1.83	0.60
1:D:144:PHE:HE2	1:D:160:GLY:HA3	1.65	0.60
1:D:95:PHE:HE2	1:D:130:LEU:HG	1.67	0.59
1:B:75:ARG:HB3	1:B:331:TRP:CZ2	2.37	0.59
1:C:276:LYS:HD3	7:C:513:HOH:O	2.01	0.59
1:B:309:ASN:HB3	1:B:327:ALA:HA	1.86	0.58
1:B:86:GLU:O	1:B:87:LEU:HD23	2.05	0.56
1:A:266:PHE:O	1:A:271:SER:HB3	2.06	0.55
1:D:310:GLN:HG3	1:D:324:ILE:HG22	1.89	0.55
1:A:75:ARG:HB3	1:A:331:TRP:CZ2	2.43	0.54
1:B:197:ILE:HG23	1:B:258:LEU:HD12	1.90	0.54
1:D:22:LEU:CD2	1:D:123:LEU:HB3	2.38	0.54
1:B:240:ASN:HA	1:B:245:HIS:ND1	2.23	0.54
1:C:80:ARG:HA	1:C:89:ILE:HD12	1.90	0.53
1:C:108:ILE:HD11	1:C:153:LEU:HD11	1.91	0.53
1:B:29:THR:HG23	1:B:131:LEU:HD11	1.91	0.53
1:B:108:ILE:HD11	1:B:153:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ASP:N	7:D:509:HOH:O	2.41	0.53
1:A:52:ASP:OD2	1:A:349:ARG:HG3	2.09	0.53
1:A:144:PHE:HE2	1:A:160:GLY:HA3	1.73	0.52
1:D:106:GLY:HA3	7:D:520:HOH:O	2.10	0.51
1:B:234:ARG:O	1:B:269:ALA:HB3	2.10	0.51
1:B:62:SER:HB3	1:B:97:LYS:HD3	1.92	0.51
1:C:265:ASP:HA	1:C:300:MET:HB3	1.92	0.51
1:A:187:ASN:OD1	1:A:233:LEU:HA	2.11	0.51
1:A:167:THR:HG22	1:A:195:VAL:HG12	1.93	0.51
1:A:116:SER:OG	1:A:118:GLN:HG3	2.11	0.50
1:A:80:ARG:HA	1:A:89:ILE:HD12	1.94	0.50
1:D:22:LEU:HD21	1:D:123:LEU:HB3	1.94	0.49
1:D:149:THR:OG1	1:D:150:PRO:HD3	2.13	0.49
1:C:23:LEU:HD23	1:C:127:ARG:CZ	2.43	0.49
1:D:310:GLN:HG2	1:D:323:SER:O	2.13	0.49
1:D:52:ASP:OD2	1:D:349:ARG:HD3	2.13	0.49
1:D:144:PHE:CE2	1:D:160:GLY:HA3	2.47	0.48
1:A:109:ASN:O	1:A:117:PHE:HA	2.13	0.48
1:A:144:PHE:CE2	1:A:160:GLY:HA3	2.48	0.48
1:B:335:ASP:O	1:B:339:ARG:HG3	2.14	0.48
1:D:17:LEU:HD11	1:D:124:ARG:NH2	2.29	0.48
1:A:234:ARG:HE	1:A:234:ARG:HB2	1.55	0.48
1:B:9:ARG:NH2	7:B:512:HOH:O	2.47	0.47
1:A:168:GLU:HG3	1:A:195:VAL:CG1	2.45	0.47
1:B:141:ALA:HB1	1:B:159:TRP:HE3	1.80	0.47
1:B:285:VAL:HG13	1:B:296:ILE:HD13	1.97	0.47
1:B:297:ILE:HD12	1:B:298:GLY:N	2.29	0.47
1:D:146:ASP:OD2	1:D:149:THR:HG23	2.14	0.46
1:C:234:ARG:NH1	1:C:235:GLY:O	2.49	0.46
1:A:246:VAL:O	1:A:250:LYS:HG3	2.15	0.46
1:B:186:LYS:HD3	1:B:234:ARG:HG2	1.96	0.46
1:A:277:LYS:O	1:A:281:VAL:HG23	2.16	0.46
1:B:70:LYS:HE2	1:B:132:ASP:CB	2.46	0.46
1:D:97:LYS:HA	1:D:97:LYS:HD2	1.70	0.46
1:B:266:PHE:O	1:B:271:SER:HB3	2.17	0.45
1:D:114:ASP:N	1:D:114:ASP:OD1	2.49	0.45
1:B:250:LYS:HD3	1:B:295:ALA:CB	2.45	0.45
1:A:224:SER:CB	1:B:11:LYS:HE3	2.47	0.45
1:A:168:GLU:HG3	1:A:195:VAL:HG13	1.99	0.45
1:A:186:LYS:HB3	1:A:234:ARG:HD2	1.99	0.45
1:D:109:ASN:O	1:D:117:PHE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ILE:HG23	1:C:231:ILE:CD1	2.47	0.44
1:A:86:GLU:HG2	1:A:346:LYS:HG3	1.98	0.44
1:D:58:ILE:HD11	1:D:334:THR:HG23	2.00	0.44
1:B:72:TYR:HE1	1:B:76:LEU:HD22	1.83	0.43
1:D:95:PHE:CZ	1:D:129:LEU:HD23	2.53	0.43
1:C:55:LEU:O	1:C:298:GLY:HA2	2.18	0.43
1:D:149:THR:N	1:D:150:PRO:CD	2.81	0.43
1:C:250:LYS:HG2	1:C:260:ALA:HB1	2.00	0.43
1:D:158:SER:O	1:D:182:PRO:HD2	2.18	0.43
1:A:241:TYR:CG	1:A:281:VAL:HG13	2.53	0.43
1:B:215:TRP:HE1	1:D:18:PRO:HD3	1.84	0.43
1:C:274:GLN:CD	1:C:277:LYS:HE3	2.39	0.43
1:B:242:SER:N	7:B:515:HOH:O	2.52	0.43
1:B:267:SER:OG	1:B:268:HIS:N	2.47	0.43
1:B:316:GLU:N	1:B:317:PRO:CD	2.82	0.42
1:C:95:PHE:HE2	1:C:130:LEU:HG	1.85	0.42
1:D:142:GLY:O	1:D:160:GLY:HA2	2.19	0.42
1:A:241:TYR:O	1:A:288:GLN:NE2	2.44	0.42
1:A:193:ILE:O	1:A:197:ILE:HG13	2.19	0.42
1:D:55:LEU:O	1:D:298:GLY:HA2	2.19	0.42
1:D:92:ARG:HG3	1:D:94:TYR:CE1	2.55	0.42
1:B:39:ALA:O	1:B:43:ILE:HG13	2.18	0.42
1:A:222:ASN:HB2	1:B:12:GLU:HG2	2.02	0.41
1:B:55:LEU:O	1:B:298:GLY:HA2	2.21	0.41
1:C:183:VAL:O	1:C:229:CYS:HA	2.19	0.41
1:D:75:ARG:HB3	1:D:331:TRP:CZ2	2.56	0.41
1:B:120:ASN:HB2	3:B:404:FLC:OG2	2.20	0.41
1:A:186:LYS:HG2	1:A:234:ARG:HG2	2.03	0.41
1:D:146:ASP:OD1	1:D:147:MET:N	2.53	0.41
1:C:9:ARG:HD2	1:D:179:LEU:O	2.21	0.41
1:D:282:CYS:O	1:D:283:ALA:C	2.58	0.41
1:A:52:ASP:OD2	1:A:349:ARG:NE	2.40	0.41
1:A:151:GLN:OE1	1:A:214:LYS:HD3	2.21	0.41
1:C:186:LYS:HB3	1:C:234:ARG:HG2	2.03	0.41
1:D:341:LEU:HD13	1:D:341:LEU:HA	1.95	0.41
1:C:57:VAL:O	1:C:300:MET:HA	2.21	0.41
1:D:95:PHE:HB3	1:D:108:ILE:HG13	2.02	0.41
1:D:106:GLY:CA	7:D:520:HOH:O	2.68	0.41
1:D:297:ILE:C	1:D:297:ILE:HD12	2.41	0.40
1:B:285:VAL:O	1:B:289:ILE:HG13	2.22	0.40
1:D:168:GLU:HA	1:D:173:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:CD1	1:B:334:THR:HG23	2.49	0.40
1:A:210:LEU:HD21	1:B:119:ILE:HG21	2.02	0.40
1:C:61:CYS:SG	1:C:326:ASP:HB2	2.61	0.40
1:D:187:ASN:OD1	1:D:233:LEU:HA	2.22	0.40

There are no symmetry-related clashes.

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	334/351 (95%)	326 (98%)	8 (2%)	0	100	100
1	B	336/351 (96%)	328 (98%)	8 (2%)	0	100	100
1	C	342/351 (97%)	336 (98%)	6 (2%)	0	100	100
1	D	331/351 (94%)	320 (97%)	10 (3%)	1 (0%)	41	37
All	All	1343/1404 (96%)	1310 (98%)	32 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	190	ASP

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	263/283 (93%)	259 (98%)	4 (2%)	65	69
1	B	257/283 (91%)	252 (98%)	5 (2%)	57	61
1	C	269/283 (95%)	266 (99%)	3 (1%)	73	78
1	D	254/283 (90%)	247 (97%)	7 (3%)	43	44
All	All	1043/1132 (92%)	1024 (98%)	19 (2%)	59	63

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	187	ASN
1	A	234	ARG
1	A	304	HIS
1	B	187	ASN
1	B	234	ARG
1	B	244	LYS
1	B	304	HIS
1	B	320	TYR
1	C	234	ARG
1	C	255	LYS
1	C	287	GLN
1	D	14	LYS
1	D	81	GLU
1	D	107	LEU
1	D	234	ARG
1	D	300	MET
1	D	304	HIS
1	D	348	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	287	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

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$
3	FLC	A	403	2	12,12,12	1.27	1 (8%)	17,17,17	2.12	3 (17%)
5	ACT	B	405	2	3,3,3	0.98	0	3,3,3	0.81	0
4	PO4	B	403	-	4,4,4	0.67	0	6,6,6	0.44	0
3	FLC	C	404	2	12,12,12	1.29	1 (8%)	17,17,17	2.35	5 (29%)
3	FLC	D	403	2	12,12,12	1.32	1 (8%)	17,17,17	2.15	6 (35%)
3	FLC	B	404	2	12,12,12	1.55	2 (16%)	17,17,17	2.14	8 (47%)
6	52L	C	401	2	17,18,18	2.45	5 (29%)	20,25,25	1.46	4 (20%)

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
3	FLC	A	403	2	-	9/16/16/16	-
3	FLC	C	404	2	-	8/16/16/16	-
3	FLC	D	403	2	-	8/16/16/16	-
3	FLC	B	404	2	-	7/16/16/16	-
6	52L	C	401	2	-	4/24/24/24	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	52L	P-O6	6.62	1.81	1.60
6	C	401	52L	C6-C5	4.49	1.58	1.51
6	C	401	52L	O27-N1	-3.30	1.30	1.40
3	B	404	FLC	CA-CB	-2.78	1.50	1.53
3	B	404	FLC	CB-CBC	-2.64	1.50	1.53
6	C	401	52L	O30-C17	-2.39	1.23	1.30
3	C	404	FLC	OHB-CB	-2.27	1.38	1.43
3	D	403	FLC	CB-CBC	-2.14	1.51	1.53
3	A	403	FLC	OG2-CGC	-2.07	1.23	1.30
6	C	401	52L	O6-C6	-2.02	1.37	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	404	FLC	OB2-CBC-CB	6.07	123.59	113.05
3	D	403	FLC	CA-CB-CBC	5.37	121.64	110.11
3	A	403	FLC	OHB-CB-CBC	-4.95	101.92	108.86
3	C	404	FLC	OHB-CB-CBC	4.82	115.62	108.86
3	A	403	FLC	OB2-CBC-CB	4.70	121.21	113.05
3	B	404	FLC	CA-CB-CBC	4.47	119.72	110.11
3	D	403	FLC	OB2-CBC-CB	3.96	119.93	113.05
3	B	404	FLC	OB2-CBC-CB	3.87	119.78	113.05
3	A	403	FLC	CG-CB-CBC	3.28	117.14	110.11
6	C	401	52L	O3P-P-O2P	2.61	117.61	107.64
6	C	401	52L	O3P-P-O6	-2.57	99.89	106.73
3	D	403	FLC	OHB-CB-CBC	-2.52	105.33	108.86
6	C	401	52L	O2P-P-O6	-2.49	100.10	106.73
3	B	404	FLC	OG2-CGC-CG	2.43	122.17	114.35
3	B	404	FLC	OA2-CAC-OA1	-2.42	117.27	123.30
3	C	404	FLC	OA2-CAC-CA	2.30	121.72	114.35
3	B	404	FLC	CB-CG-CGC	-2.24	108.40	113.81
3	C	404	FLC	OG2-CGC-CG	2.21	121.45	114.35
3	D	403	FLC	CB-CG-CGC	-2.18	108.54	113.81
3	D	403	FLC	OA2-CAC-OA1	-2.18	117.87	123.30
3	C	404	FLC	OB2-CBC-OB1	-2.15	116.97	123.82
3	B	404	FLC	OHB-CB-CBC	-2.13	105.88	108.86
3	B	404	FLC	OB1-CBC-CB	-2.11	119.26	122.25
3	D	403	FLC	OG2-CGC-CG	2.07	120.99	114.35
3	B	404	FLC	OG2-CGC-OG1	-2.05	118.19	123.30
6	C	401	52L	O3-C3-C4	2.03	114.05	109.10

There are no chirality outliers.

All (36) torsion outliers are listed below:

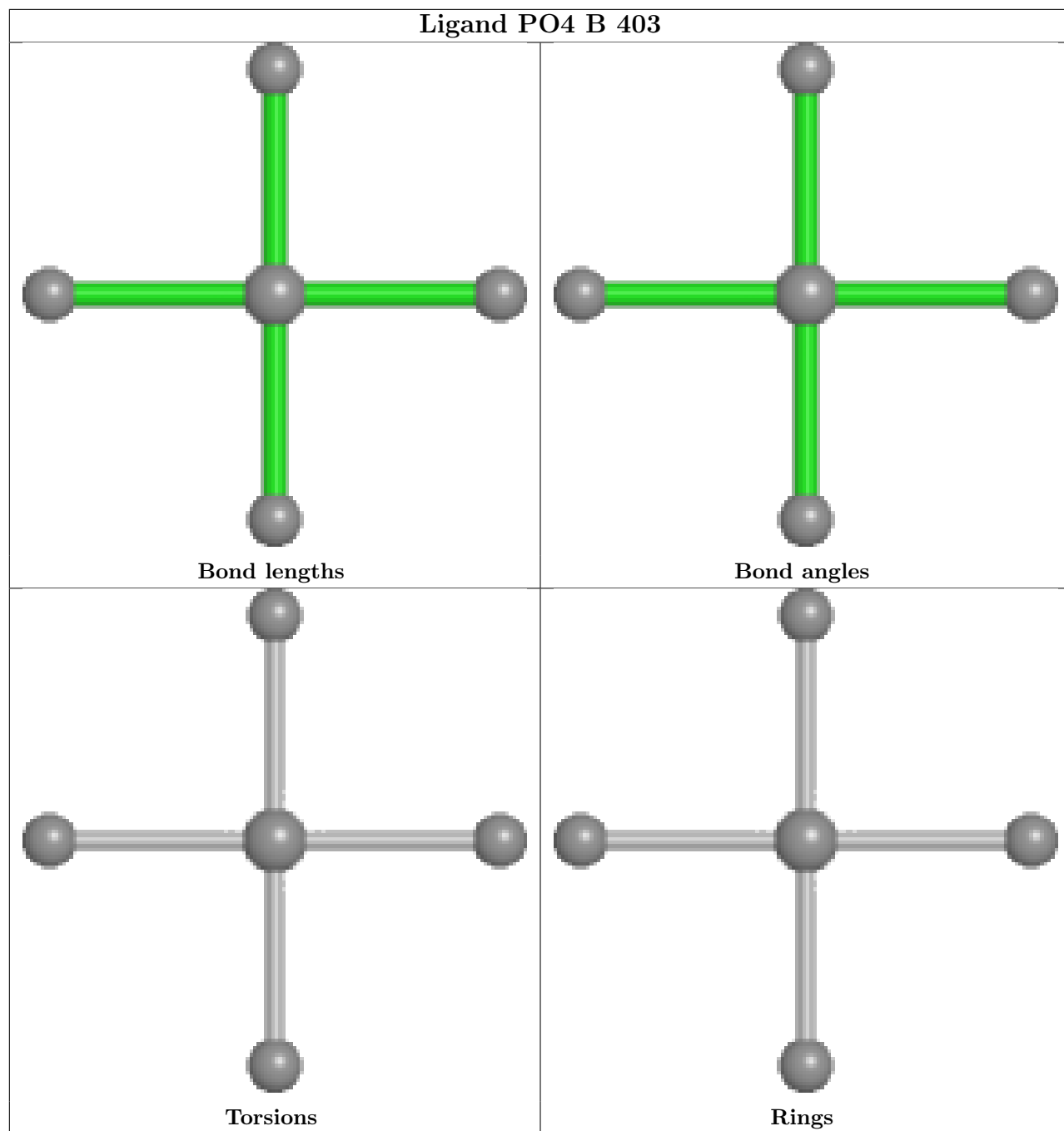
Mol	Chain	Res	Type	Atoms
3	A	403	FLC	CA-CB-CBC-OB1
3	A	403	FLC	CA-CB-CBC-OB2
3	A	403	FLC	OHB-CB-CBC-OB1
3	A	403	FLC	OHB-CB-CBC-OB2
3	B	404	FLC	CA-CB-CG-CGC
3	B	404	FLC	CBC-CB-CG-CGC
3	B	404	FLC	OHB-CB-CG-CGC
3	C	404	FLC	CA-CB-CBC-OB1
3	C	404	FLC	CA-CB-CBC-OB2
3	C	404	FLC	OHB-CB-CBC-OB1
3	C	404	FLC	OHB-CB-CBC-OB2
3	D	403	FLC	CBC-CB-CG-CGC
6	C	401	52L	C2-C1-C17-O30
3	B	404	FLC	CAC-CA-CB-CBC
3	B	404	FLC	CAC-CA-CB-OHB
3	D	403	FLC	CAC-CA-CB-CBC
3	D	403	FLC	CAC-CA-CB-OHB
3	A	403	FLC	CA-CB-CG-CGC
3	D	403	FLC	CA-CB-CG-CGC
3	A	403	FLC	CG-CB-CBC-OB2
3	D	403	FLC	CG-CB-CBC-OB2
3	A	403	FLC	OHB-CB-CG-CGC
3	B	404	FLC	CAC-CA-CB-CG
3	D	403	FLC	OHB-CB-CG-CGC
3	D	403	FLC	CAC-CA-CB-CG
3	A	403	FLC	CG-CB-CBC-OB1
3	C	404	FLC	CG-CB-CBC-OB2
3	D	403	FLC	CG-CB-CBC-OB1
3	A	403	FLC	CAC-CA-CB-OHB
3	C	404	FLC	CG-CB-CBC-OB1
3	C	404	FLC	CB-CA-CAC-OA1
3	C	404	FLC	CB-CA-CAC-OA2
6	C	401	52L	N1-C1-C17-O30
6	C	401	52L	N1-C1-C17-O29
3	B	404	FLC	CA-CB-CBC-OB1
6	C	401	52L	C3-C4-C5-O5

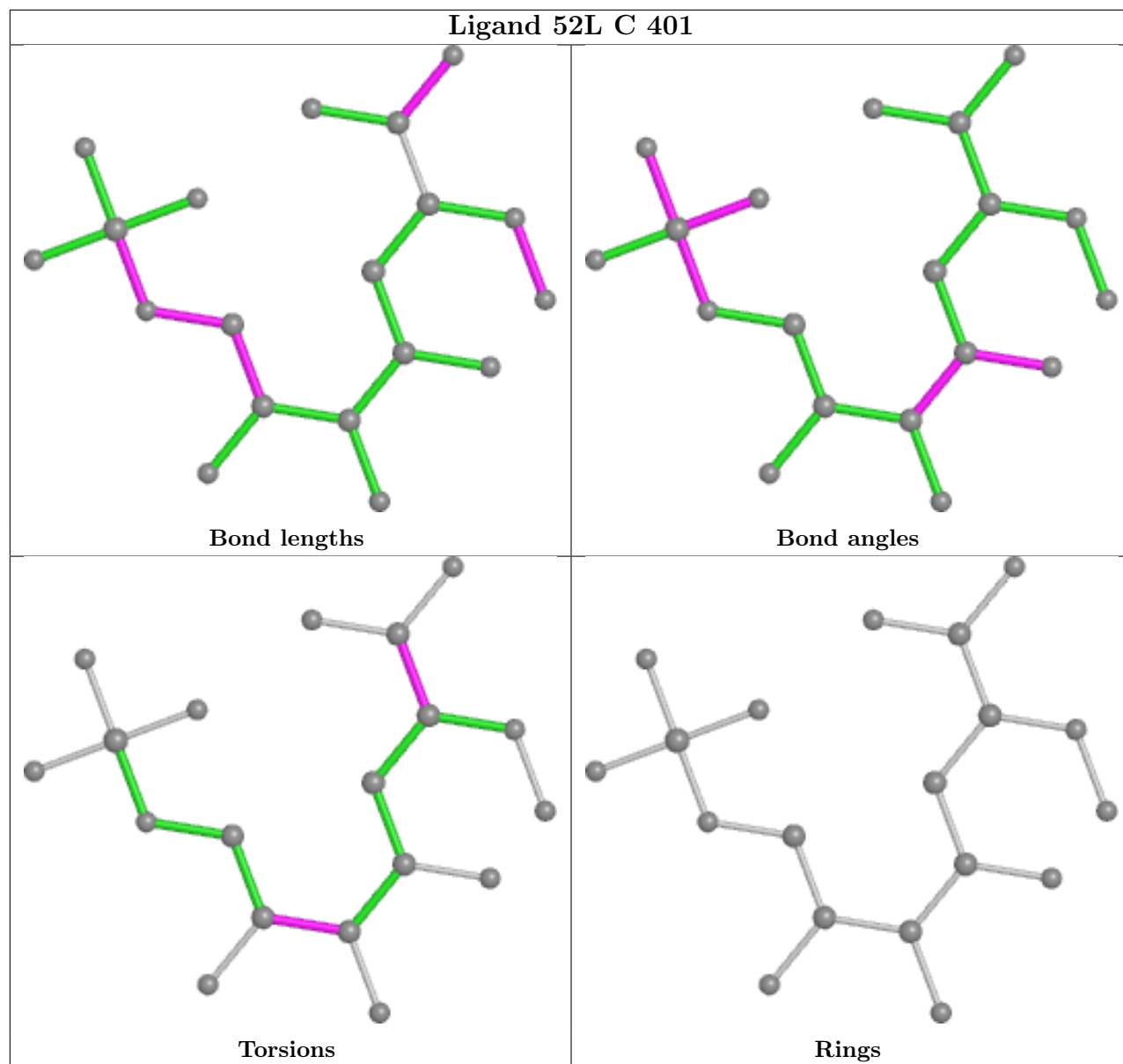
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	FLC	1	0
3	B	404	FLC	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.





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

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	339/351 (96%)	0.08	9 (2%) 54 53	20, 36, 53, 58	0
1	B	340/351 (96%)	0.21	15 (4%) 34 33	29, 51, 66, 73	0
1	C	344/351 (98%)	-0.27	1 (0%) 94 93	15, 24, 37, 51	0
1	D	336/351 (95%)	0.26	28 (8%) 11 10	24, 46, 58, 71	0
All	All	1359/1404 (96%)	0.07	53 (3%) 39 38	15, 39, 61, 73	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	350	GLY	6.3
1	D	236	GLY	4.9
1	A	271	SER	4.9
1	D	238	GLU	4.7
1	D	269	ALA	4.7
1	D	272	SER	4.5
1	A	350	GLY	4.1
1	D	104	TRP	4.1
1	D	274	GLN	4.0
1	B	254	ASN	3.8
1	B	292	GLY	3.7
1	D	251	GLU	3.6
1	A	269	ALA	3.5
1	D	191	GLY	3.3
1	D	192	THR	3.3
1	C	350	GLY	3.2
1	B	289	ILE	3.2
1	D	271	SER	3.2
1	B	244	LYS	3.1
1	B	291	GLY	3.0
1	B	347	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	100	THR	2.9
1	A	38	HIS	2.9
1	A	238	GLU	2.9
1	D	254	ASN	2.8
1	A	272	SER	2.8
1	D	311	SER	2.8
1	D	188	GLY	2.8
1	D	268	HIS	2.7
1	B	29	THR	2.6
1	B	316	GLU	2.6
1	D	270	ASN	2.6
1	B	247	ALA	2.5
1	A	270	ASN	2.5
1	D	287	GLN	2.5
1	D	273	LYS	2.4
1	D	291	GLY	2.4
1	B	290	ALA	2.4
1	B	248	GLU	2.3
1	D	105	LYS	2.3
1	B	271	SER	2.3
1	D	237	LYS	2.2
1	D	189	THR	2.2
1	D	245	HIS	2.2
1	D	256	ALA	2.2
1	A	273	LYS	2.1
1	B	48	LYS	2.1
1	B	251	GLU	2.0
1	A	268	HIS	2.0
1	D	252	GLY	2.0
1	B	317	PRO	2.0
1	D	98	PRO	2.0
1	D	96	GLU	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

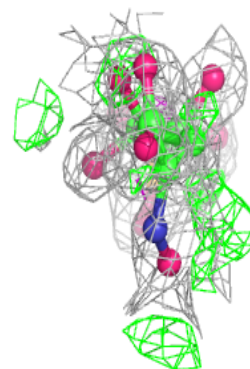
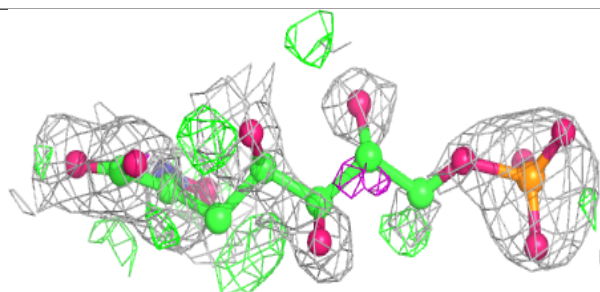
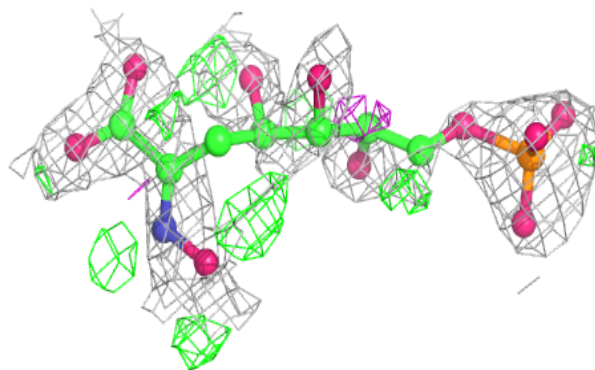
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FLC	D	403	13/13	0.77	0.32	44,56,62,69	0
3	FLC	B	404	13/13	0.81	0.33	49,57,66,78	0
3	FLC	A	403	13/13	0.82	0.30	32,48,67,71	0
5	ACT	B	405	4/4	0.83	0.19	57,62,69,69	0
6	52L	C	401	19/19	0.86	0.24	23,30,39,41	19
2	PR	A	401	1/1	0.91	0.22	54,54,54,54	1
3	FLC	C	404	13/13	0.92	0.20	34,40,56,58	0
2	PR	B	402	1/1	0.96	0.07	56,56,56,56	0
4	PO4	B	403	5/5	0.96	0.11	57,63,65,69	0
2	PR	C	403	1/1	0.97	0.12	46,46,46,46	0
2	PR	D	402	1/1	0.97	0.06	57,57,57,57	0
2	PR	B	401	1/1	0.97	0.13	57,57,57,57	1
2	PR	D	401	1/1	0.98	0.07	64,64,64,64	1
2	PR	C	402	1/1	0.98	0.13	24,24,24,24	1
2	PR	A	402	1/1	0.98	0.06	42,42,42,42	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.

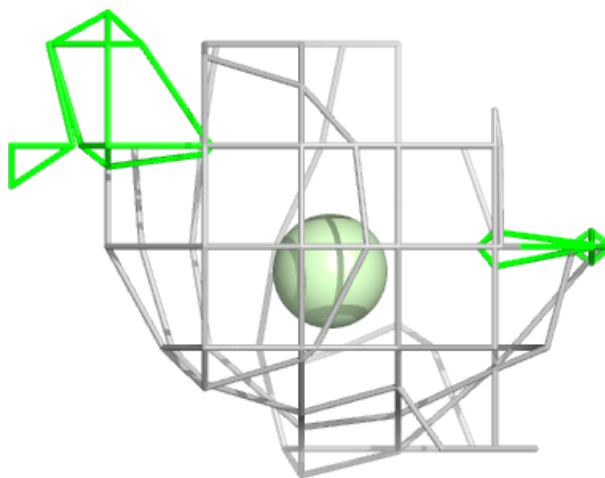
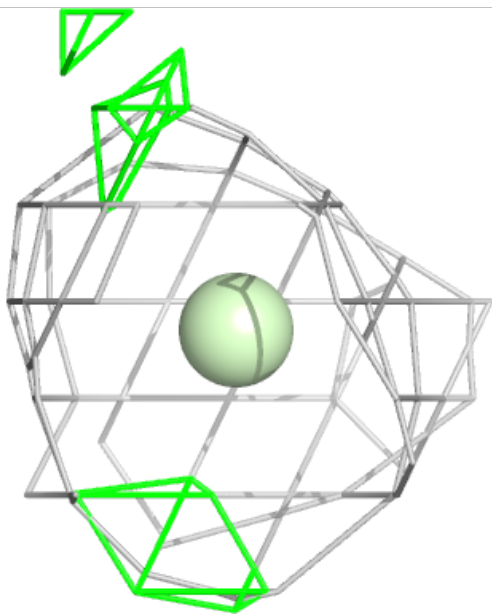
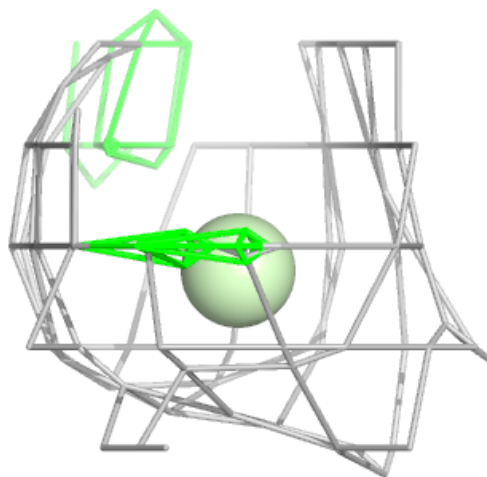
Electron density around 52L C 401:

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



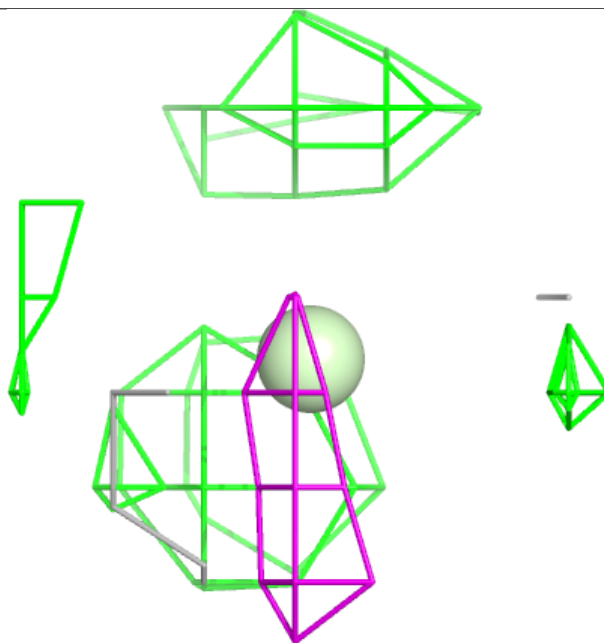
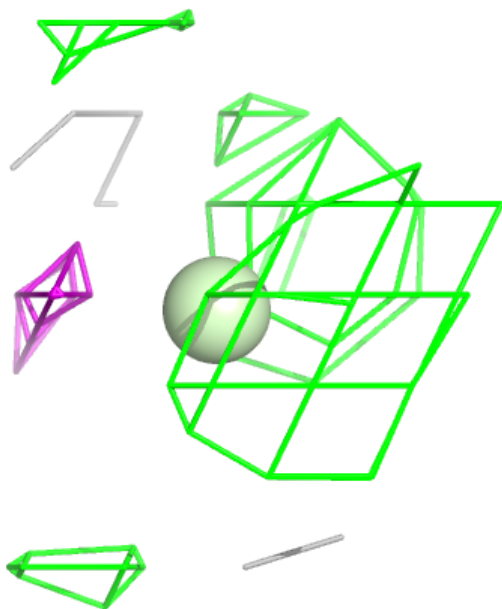
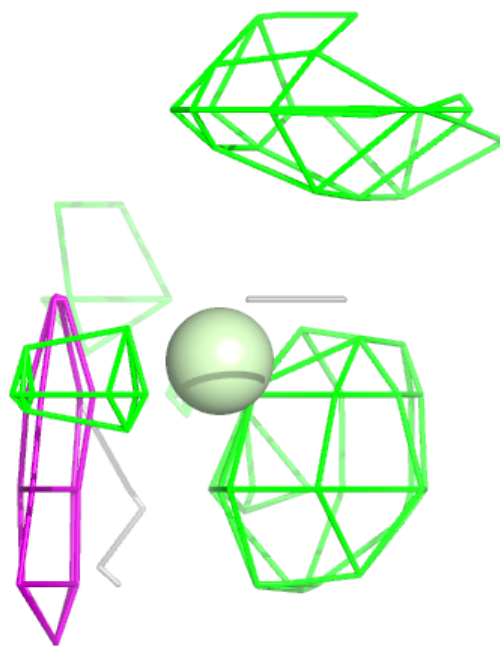
Electron density around PR A 401:

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



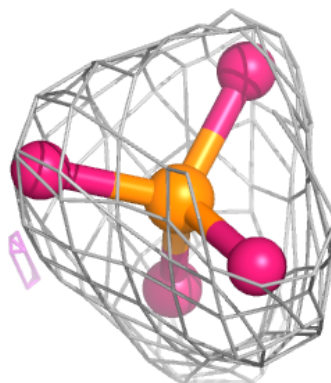
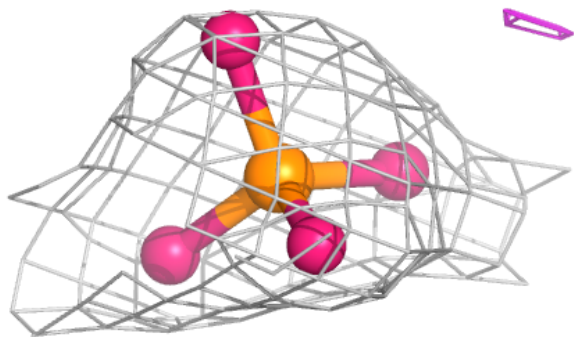
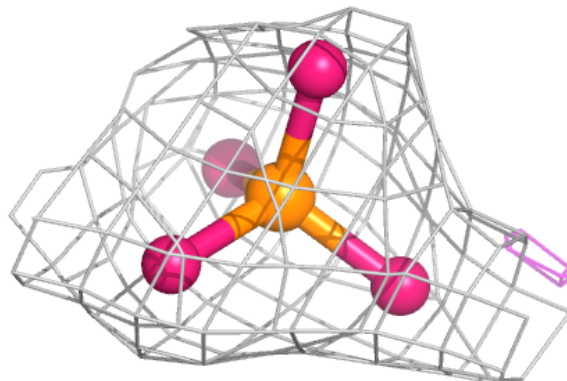
Electron density around PR B 402:

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



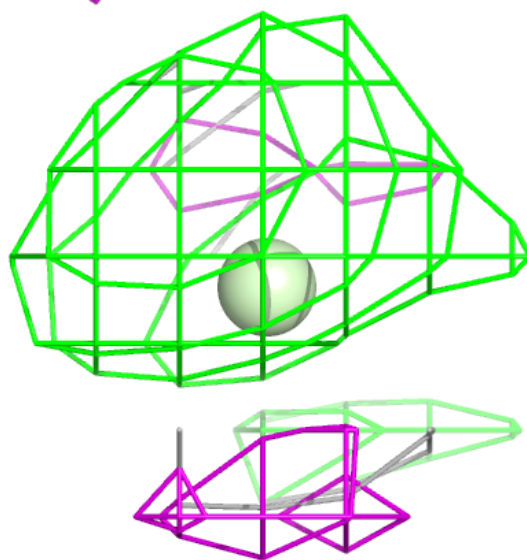
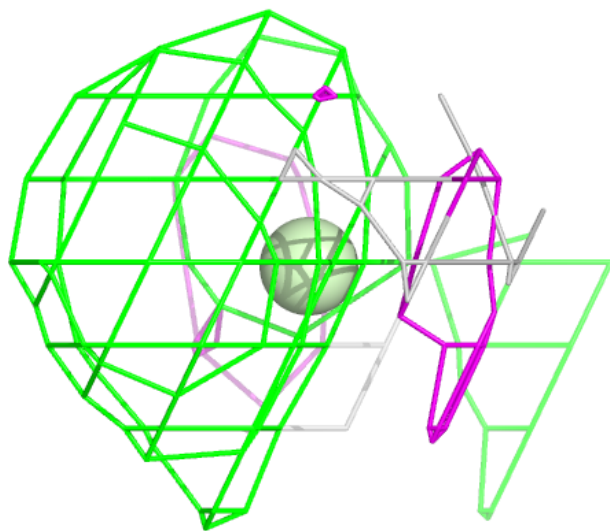
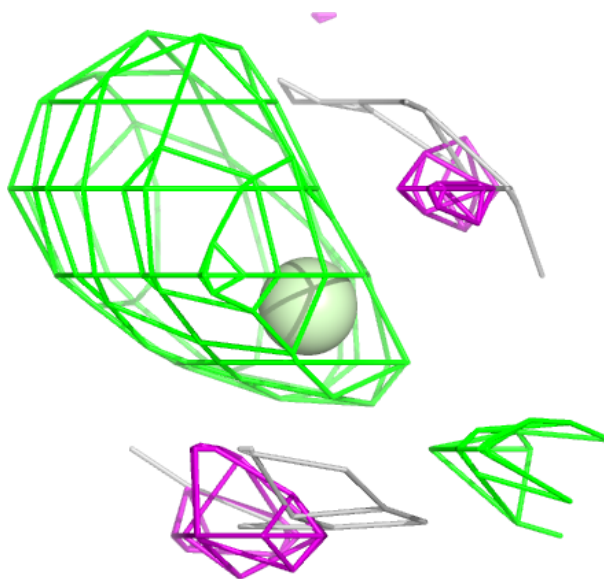
Electron density around PO4 B 403:

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



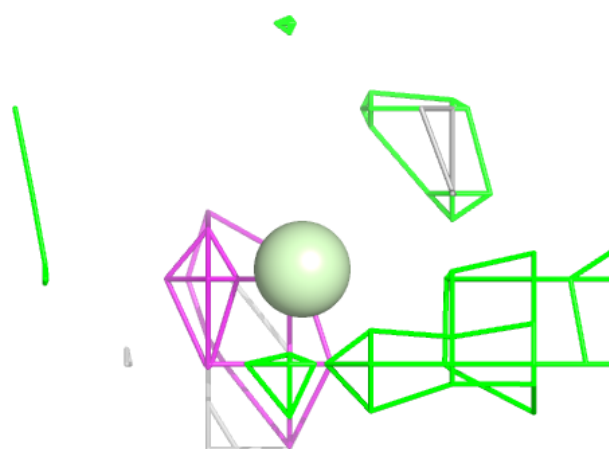
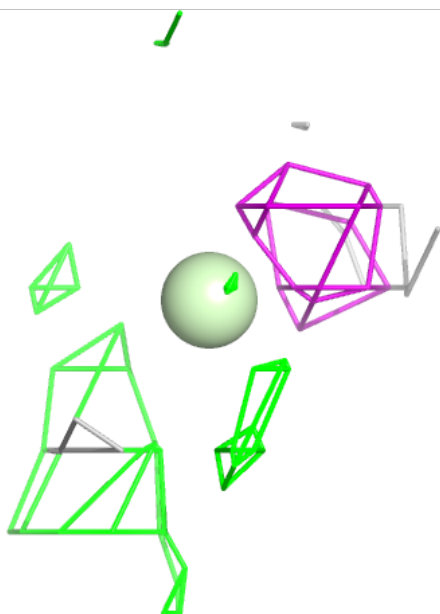
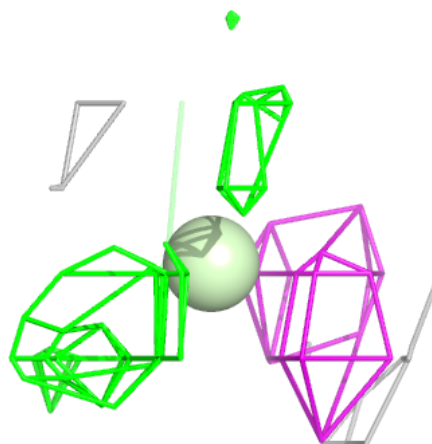
Electron density around PR C 403:

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



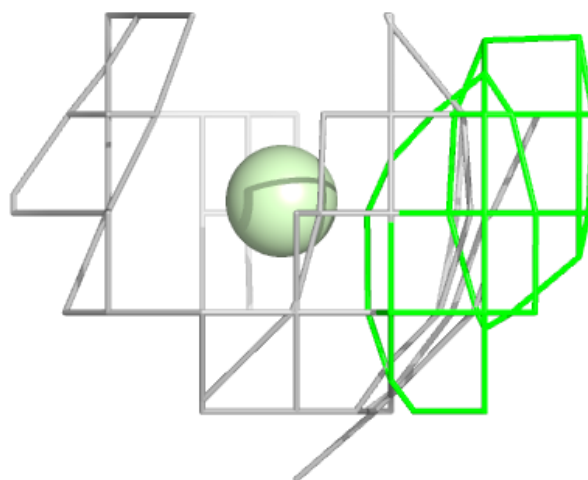
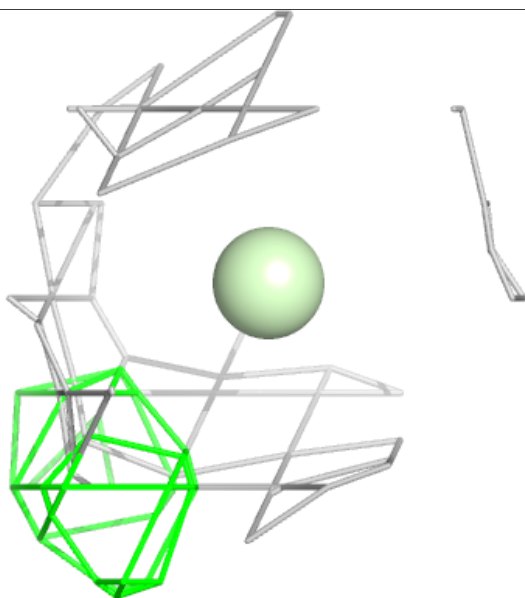
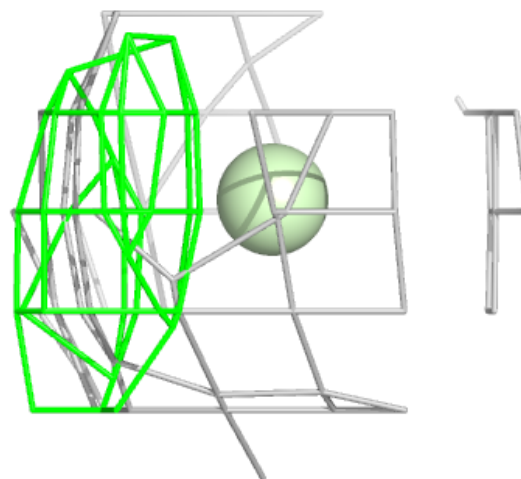
Electron density around PR D 402:

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



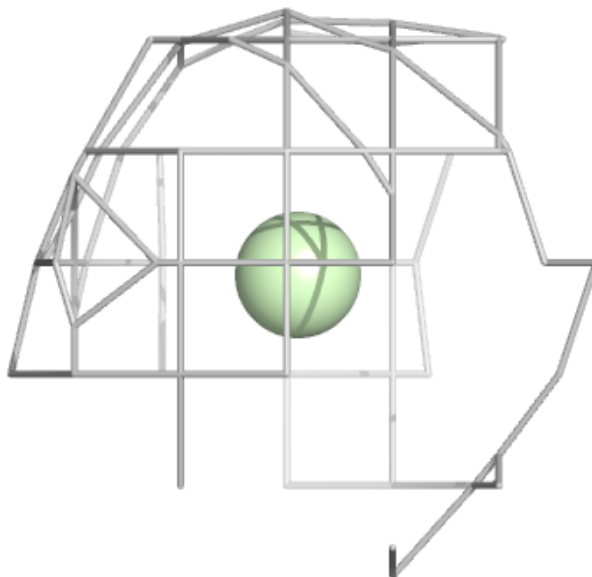
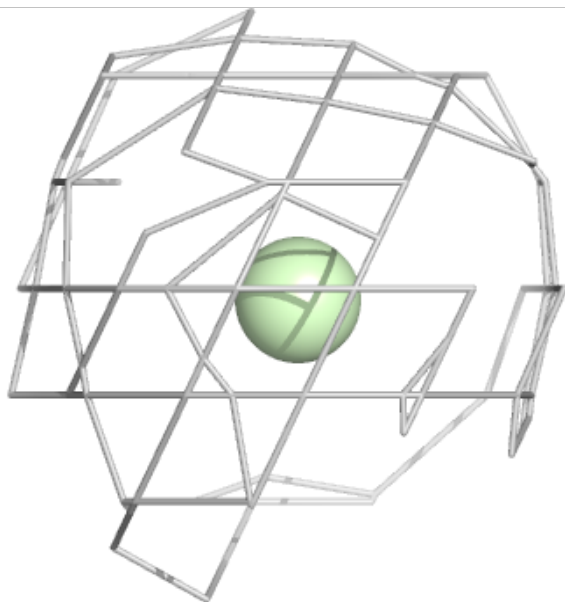
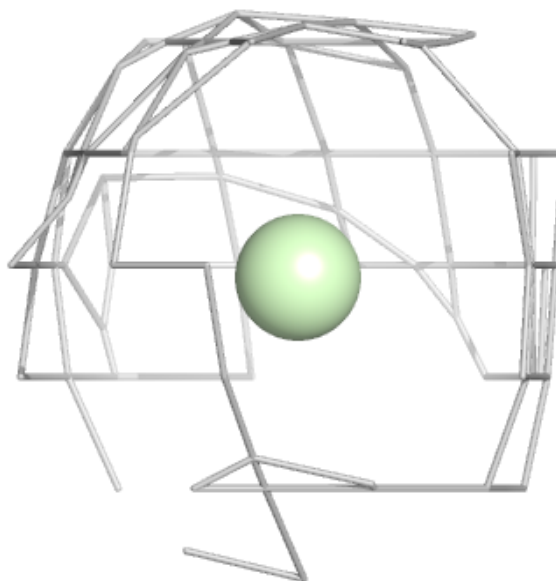
Electron density around PR B 401:

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



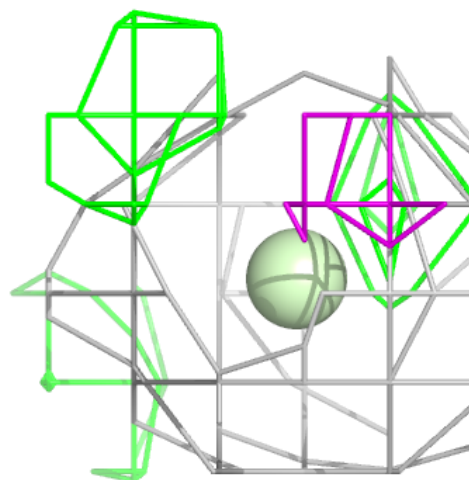
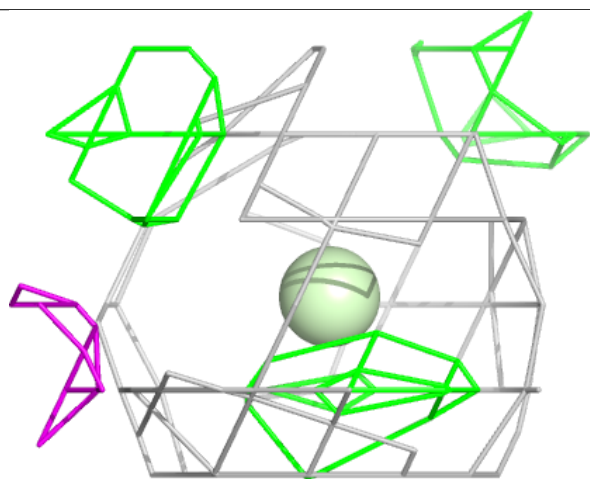
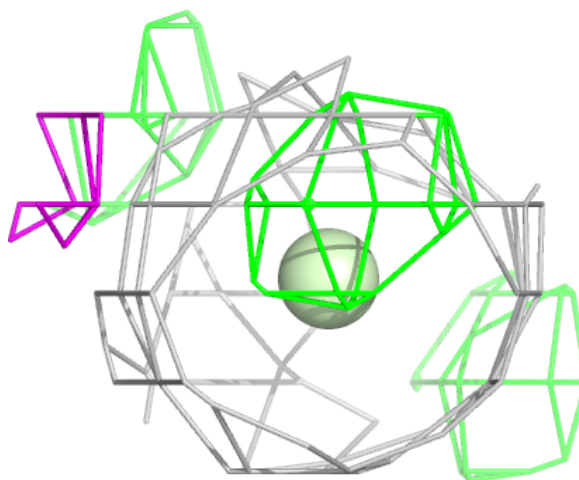
Electron density around PR D 401:

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



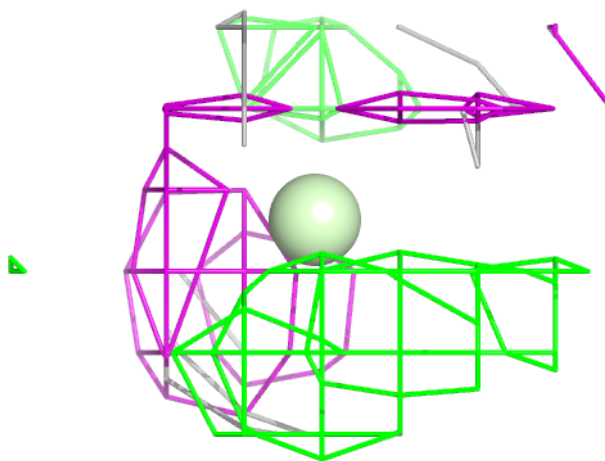
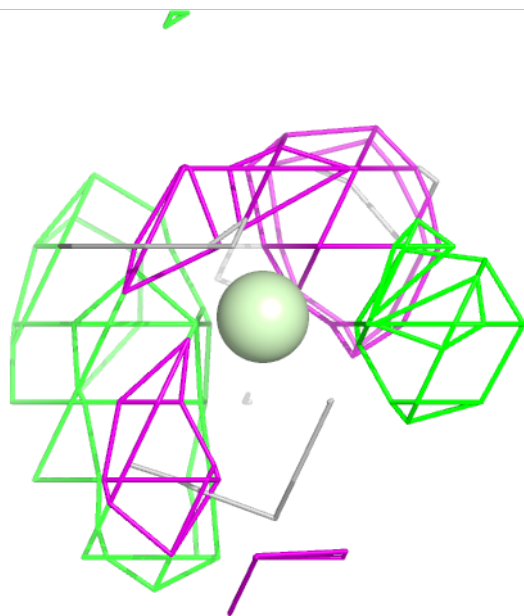
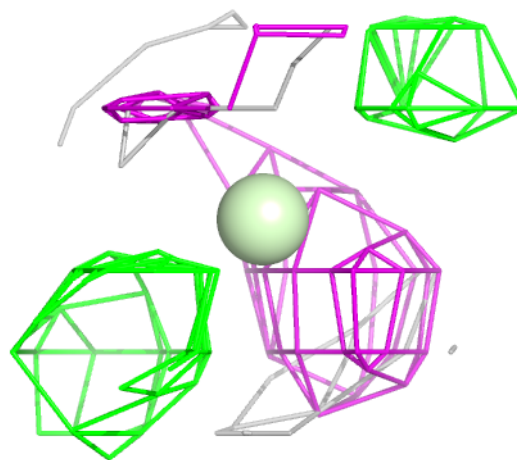
Electron density around PR C 402:

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



Electron density around PR A 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.