



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:27 AM BST

PDB ID : 6N0Z  
Title : Crystal structure of Anaerolinea thermophila mevalonate 5-phosphate decarboxylase N20K H194M mutant complexed with (R)-MVAPP  
Authors : Noel, J.P.; Thomas, S.T.; Louie, G.V.  
Deposited on : 2018-11-07  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

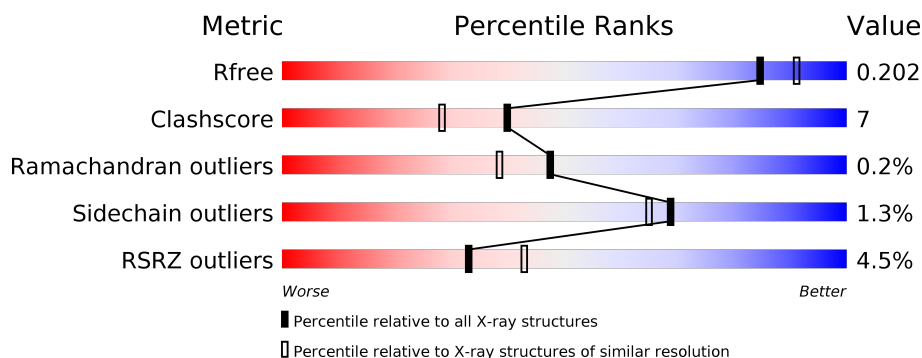
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	330	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div></div> </div> <div></div> </div>
1	B	330	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div></div> </div> <div></div> </div>
1	C	330	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div></div> </div> <div></div> </div>
1	D	330	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	E	330	<div> <div>10%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	F	330	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16769 atoms, of which 60 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 Diphosphomevalonate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2459	1557	431	459	12			
1	B	327	Total	C	N	O	S	0	0	0
			2488	1573	437	466	12			
1	C	327	Total	C	N	O	S	0	0	0
			2487	1573	435	467	12			
1	D	325	Total	C	N	O	S	0	0	0
			2475	1566	435	462	12			
1	E	321	Total	C	N	O	S	0	0	0
			2447	1550	429	457	11			
1	F	327	Total	C	N	O	S	0	0	0
			2491	1576	436	467	12			

There are 36 discrepancies between the modelled and reference sequences:

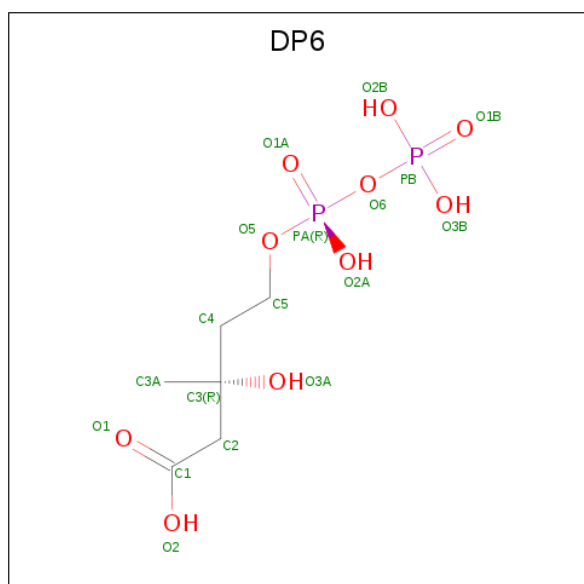
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP E8N6F3
A	-2	SER	-	expression tag	UNP E8N6F3
A	-1	HIS	-	expression tag	UNP E8N6F3
A	0	GLY	-	expression tag	UNP E8N6F3
A	20	LYS	ASN	engineered mutation	UNP E8N6F3
A	194	MET	HIS	engineered mutation	UNP E8N6F3
B	-3	GLY	-	expression tag	UNP E8N6F3
B	-2	SER	-	expression tag	UNP E8N6F3
B	-1	HIS	-	expression tag	UNP E8N6F3
B	0	GLY	-	expression tag	UNP E8N6F3
B	20	LYS	ASN	engineered mutation	UNP E8N6F3
B	194	MET	HIS	engineered mutation	UNP E8N6F3
C	-3	GLY	-	expression tag	UNP E8N6F3
C	-2	SER	-	expression tag	UNP E8N6F3
C	-1	HIS	-	expression tag	UNP E8N6F3
C	0	GLY	-	expression tag	UNP E8N6F3
C	20	LYS	ASN	engineered mutation	UNP E8N6F3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	194	MET	HIS	engineered mutation	UNP E8N6F3
D	-3	GLY	-	expression tag	UNP E8N6F3
D	-2	SER	-	expression tag	UNP E8N6F3
D	-1	HIS	-	expression tag	UNP E8N6F3
D	0	GLY	-	expression tag	UNP E8N6F3
D	20	LYS	ASN	engineered mutation	UNP E8N6F3
D	194	MET	HIS	engineered mutation	UNP E8N6F3
E	-3	GLY	-	expression tag	UNP E8N6F3
E	-2	SER	-	expression tag	UNP E8N6F3
E	-1	HIS	-	expression tag	UNP E8N6F3
E	0	GLY	-	expression tag	UNP E8N6F3
E	20	LYS	ASN	engineered mutation	UNP E8N6F3
E	194	MET	HIS	engineered mutation	UNP E8N6F3
F	-3	GLY	-	expression tag	UNP E8N6F3
F	-2	SER	-	expression tag	UNP E8N6F3
F	-1	HIS	-	expression tag	UNP E8N6F3
F	0	GLY	-	expression tag	UNP E8N6F3
F	20	LYS	ASN	engineered mutation	UNP E8N6F3
F	194	MET	HIS	engineered mutation	UNP E8N6F3

- Molecule 2 is (3R)-3-HYDROXY-5-{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}-3-METHYLPENTANOIC ACID (three-letter code: DP6) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			28	6	10	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	O	P	0	0
			28	6	10	10	2		
2	C	1	Total	C	H	O	P	0	0
			28	6	10	10	2		
2	D	1	Total	C	H	O	P	0	0
			28	6	10	10	2		
2	E	1	Total	C	H	O	P	0	0
			28	6	10	10	2		
2	F	1	Total	C	H	O	P	0	0
			28	6	10	10	2		

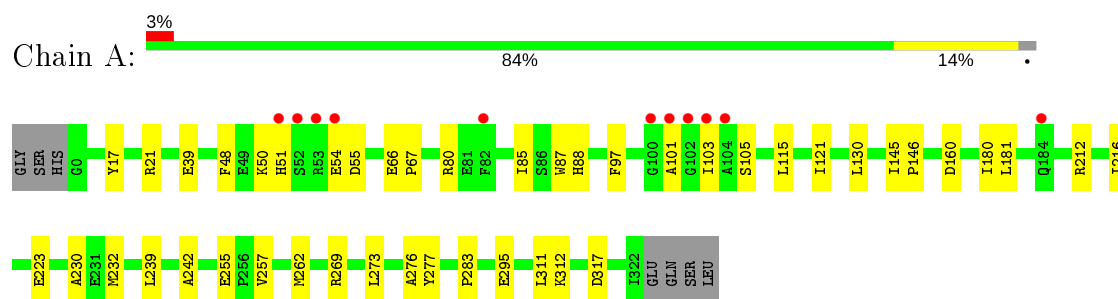
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	310	Total	O	0	0
			310	310		
3	B	312	Total	O	0	0
			312	312		
3	C	324	Total	O	0	0
			324	324		
3	D	293	Total	O	0	0
			293	293		
3	E	256	Total	O	0	0
			256	256		
3	F	259	Total	O	0	0
			259	259		

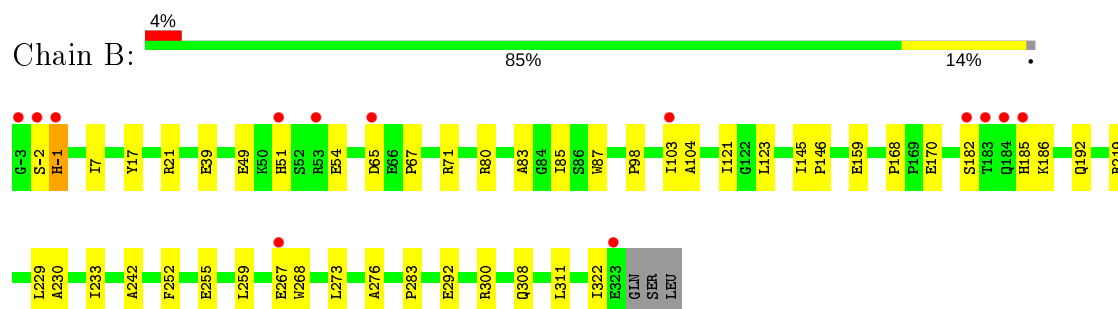
### 3 Residue-property plots [i](#)

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.

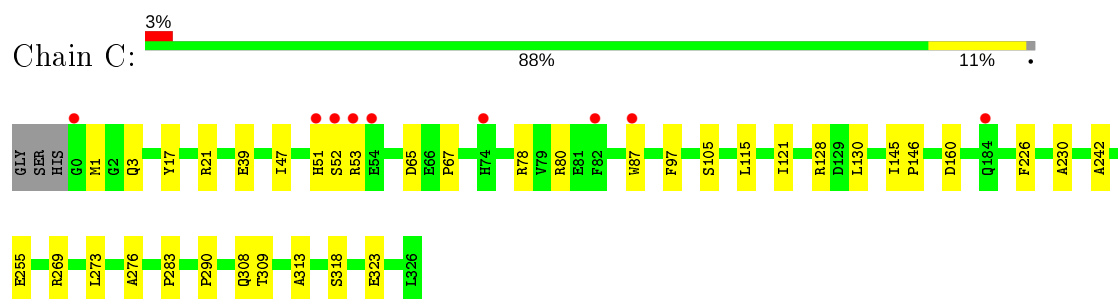
- Molecule 1: Diphosphomevalonate decarboxylase



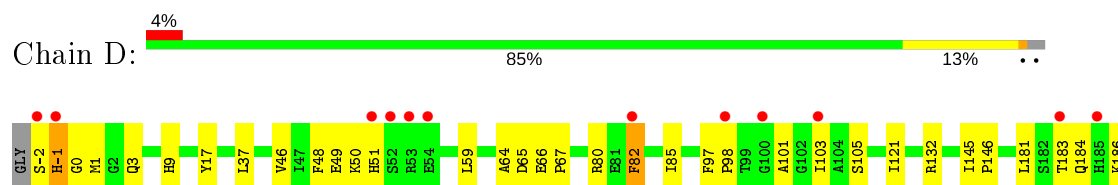
- Molecule 1: Diphosphomevalonate decarboxylase



- Molecule 1: Diphosphomevalonate decarboxylase

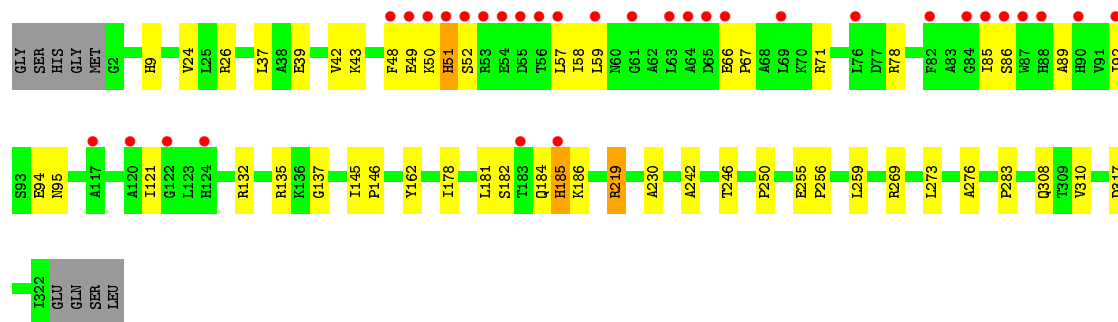
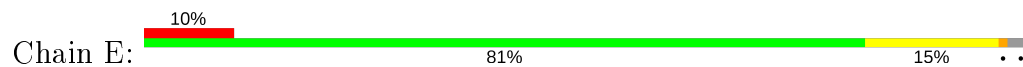


- Molecule 1: Diphosphomevalonate decarboxylase

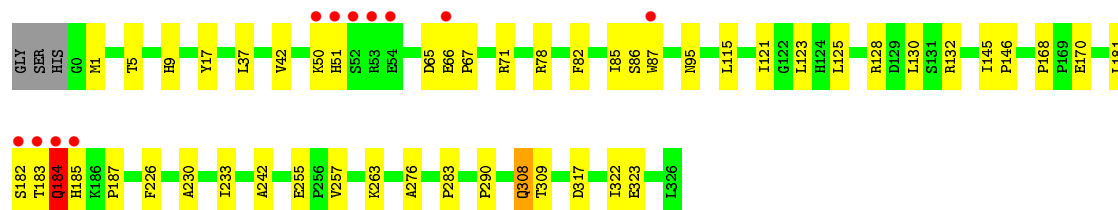
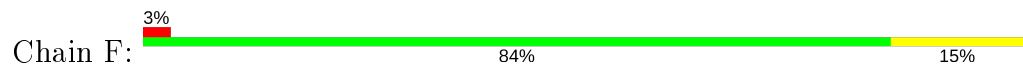




- Molecule 1: Diphosphomevalonate decarboxylase



- Molecule 1: Diphosphomevalonate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.80Å 138.09Å 105.13Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	45.57 – 1.95 45.57 – 1.95	Depositor EDS
% Data completeness (in resolution range)	78.9 (45.57-1.95) 78.9 (45.57-1.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, $R_{free}$	0.167 , 0.202 0.168 , 0.202	Depositor DCC
$R_{free}$ test set	6584 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DP6

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	0.38	0/2515	0.54	0/3423
1	B	0.39	0/2545	0.55	0/3463
1	C	0.40	0/2543	0.56	0/3462
1	D	0.37	0/2532	0.55	0/3446
1	E	0.37	0/2503	0.54	0/3408
1	F	0.37	0/2547	0.54	0/3466
All	All	0.38	0/15185	0.55	0/20668

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	219	ARG	Sidechain
1	F	184	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2459	0	2465	33	0
1	B	2488	0	2486	45	0
1	C	2487	0	2484	31	0
1	D	2475	0	2477	41	0
1	E	2447	0	2450	39	0
1	F	2491	0	2495	35	0
2	A	18	10	10	0	0
2	B	18	10	10	0	0
2	C	18	10	10	0	0
2	D	18	10	10	0	0
2	E	18	10	10	0	0
2	F	18	10	10	0	0
3	A	310	0	0	9	0
3	B	312	0	0	10	0
3	C	324	0	0	10	0
3	D	293	0	0	2	0
3	E	256	0	0	3	0
3	F	259	0	0	1	0
All	All	16709	60	14917	218	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 7.

All (218) 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:A:223:GLU:HG2	3:A:573:HOH:O	1.55	1.07
1:B:186:LYS:HE3	1:B:186:LYS:HA	1.40	1.00
1:F:183:THR:HG21	1:F:255:GLU:CD	1.85	0.97
1:D:181:LEU:HD12	1:D:283:PRO:HB2	1.50	0.91
1:B:-1:HIS:HB3	1:B:49:GLU:OE1	1.75	0.87
1:E:50:LYS:HD3	1:E:51:HIS:HB2	1.61	0.80
1:C:308:GLN:HG2	1:C:309:THR:HG23	1.63	0.79
1:A:101:ALA:HB1	1:A:180:ILE:HD12	1.65	0.78
1:D:218:ARG:O	1:D:222:LEU:HD23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-2:SER:O	1:B:-1:HIS:HB2	1.84	0.77
1:F:183:THR:HG21	1:F:255:GLU:CG	2.18	0.73
1:D:85:ILE:CD1	1:D:121:ILE:HD11	2.19	0.72
1:D:85:ILE:HG12	1:D:121:ILE:HD11	1.71	0.72
1:C:1:MET:HA	1:C:1:MET:CE	2.20	0.71
1:D:1:MET:HE3	1:D:50:LYS:HB2	1.71	0.71
1:B:219:ARG:NH2	3:B:502:HOH:O	2.24	0.71
1:B:85:ILE:HD12	1:B:121:ILE:HG12	1.72	0.70
1:B:186:LYS:CA	1:B:186:LYS:HE3	2.21	0.69
1:C:1:MET:HA	1:C:1:MET:HE3	1.75	0.67
1:D:-1:HIS:CE1	1:D:51:HIS:H	2.13	0.67
1:D:132:ARG:NH2	3:D:505:HOH:O	2.27	0.67
1:A:80:ARG:HH21	1:A:88:HIS:HA	1.60	0.67
1:E:181:LEU:HD12	1:E:283:PRO:HB2	1.76	0.66
1:E:66:GLU:HB3	1:E:67:PRO:HD3	1.76	0.66
1:D:65:ASP:OD2	1:D:67:PRO:HD2	1.97	0.65
1:F:323:GLU:HG2	3:F:599:HOH:O	1.96	0.65
1:D:85:ILE:CG1	1:D:121:ILE:HD11	2.26	0.65
1:B:-1:HIS:NE2	1:B:51:HIS:HB2	2.12	0.65
1:D:97:PHE:CE2	1:D:105:SER:HB3	2.32	0.64
1:A:55:ASP:OD1	1:A:80:ARG:NH2	2.31	0.64
1:F:255:GLU:HG2	1:F:283:PRO:HB3	1.79	0.64
1:D:80:ARG:HG2	1:D:85:ILE:CD1	2.27	0.64
1:A:262:MET:HE3	1:A:277:TYR:CE1	2.33	0.64
1:F:308:GLN:HG2	1:F:309:THR:N	2.13	0.64
1:E:57:LEU:O	1:E:58:ILE:HD13	1.98	0.63
1:B:-2:SER:O	1:B:-1:HIS:CB	2.47	0.63
1:D:-1:HIS:NE2	1:D:49:GLU:HB3	2.13	0.63
1:D:85:ILE:HD11	1:D:121:ILE:HD11	1.81	0.63
1:B:267:GLU:OE1	1:B:268:TRP:HD1	1.82	0.63
1:B:267:GLU:CD	3:B:504:HOH:O	2.35	0.62
1:B:219:ARG:CZ	3:B:502:HOH:O	2.49	0.61
1:D:1:MET:HE1	1:D:50:LYS:HD2	1.83	0.61
1:F:183:THR:HG21	1:F:255:GLU:HG3	1.83	0.61
1:C:255:GLU:HG2	1:C:283:PRO:HB3	1.83	0.60
1:D:230:ALA:HB1	1:D:276:ALA:HB2	1.84	0.60
1:B:186:LYS:HA	1:B:186:LYS:CE	2.14	0.60
1:B:85:ILE:HG21	1:B:87:TRP:CE3	2.37	0.59
1:D:218:ARG:O	1:D:222:LEU:CD2	2.51	0.59
1:E:57:LEU:HD11	1:E:59:LEU:HD21	1.85	0.59
1:F:230:ALA:HB1	1:F:276:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD13	1:A:257:VAL:HB	1.86	0.58
1:D:80:ARG:HG2	1:D:85:ILE:HD12	1.85	0.58
1:A:212:ARG:HD2	3:A:524:HOH:O	2.04	0.58
1:E:50:LYS:HD3	1:E:51:HIS:CB	2.32	0.57
1:E:42:VAL:HG22	1:E:95:ASN:HB3	1.86	0.57
1:E:219:ARG:NH2	3:E:506:HOH:O	2.37	0.57
1:B:267:GLU:CG	3:B:504:HOH:O	2.51	0.56
1:A:85:ILE:HG21	1:A:87:TRP:CE3	2.40	0.56
1:A:55:ASP:CG	1:A:80:ARG:HH22	2.08	0.56
1:C:230:ALA:HB1	1:C:276:ALA:HB2	1.88	0.56
1:D:-1:HIS:CE1	1:D:49:GLU:HB3	2.41	0.56
1:A:80:ARG:NH2	1:A:88:HIS:HA	2.21	0.56
1:E:43:LYS:HE2	1:E:94:GLU:HG2	1.87	0.56
1:D:255:GLU:HG2	1:D:283:PRO:HB3	1.88	0.56
1:D:98:PRO:HG2	1:D:311:LEU:HD11	1.87	0.56
1:C:145:ILE:HB	1:C:146:PRO:HD3	1.88	0.55
1:F:185:HIS:CE1	1:F:187:PRO:HA	2.42	0.55
1:B:-1:HIS:CD2	1:B:51:HIS:H	2.24	0.55
1:E:49:GLU:HB2	1:E:52:SER:OG	2.07	0.55
1:E:145:ILE:HB	1:E:146:PRO:HD3	1.88	0.54
1:E:85:ILE:HD12	1:E:121:ILE:HG12	1.88	0.54
1:A:54:GLU:N	1:A:54:GLU:OE1	2.40	0.54
1:B:104:ALA:HB1	3:B:597:HOH:O	2.07	0.54
1:F:308:GLN:HG2	1:F:309:THR:H	1.72	0.54
1:A:115:LEU:HD13	1:A:130:LEU:HD11	1.90	0.54
1:D:1:MET:CE	1:D:50:LYS:HD2	2.38	0.54
1:E:255:GLU:HG2	1:E:283:PRO:HB3	1.90	0.54
1:F:128:ARG:O	1:F:132:ARG:HG3	2.07	0.54
1:C:242:ALA:HB1	1:D:242:ALA:HB1	1.88	0.54
1:B:267:GLU:HG2	3:B:538:HOH:O	2.08	0.53
1:A:103:ILE:HD11	1:A:311:LEU:HD12	1.91	0.53
1:C:128:ARG:CD	3:C:503:HOH:O	2.57	0.53
1:F:145:ILE:HB	1:F:146:PRO:HD3	1.91	0.52
1:C:65:ASP:OD1	1:C:67:PRO:HD2	2.09	0.52
1:C:121:ILE:O	1:C:121:ILE:HG22	2.09	0.52
1:E:132:ARG:HG2	1:E:162:TYR:HB3	1.91	0.52
1:B:65:ASP:OD2	1:B:67:PRO:HD2	2.10	0.52
1:D:-2:SER:HB3	1:D:0:GLY:H	1.75	0.51
1:D:85:ILE:C	1:D:85:ILE:HD12	2.30	0.51
1:C:115:LEU:HD13	1:C:130:LEU:HD21	1.92	0.51
1:E:85:ILE:HG22	1:E:86:SER:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:LEU:HD22	1:B:300:ARG:CZ	2.41	0.51
1:E:50:LYS:CD	1:E:51:HIS:HB2	2.37	0.51
1:A:242:ALA:HB1	1:E:242:ALA:HB1	1.93	0.50
1:C:128:ARG:NH1	3:C:503:HOH:O	2.23	0.50
1:C:80:ARG:NE	3:C:513:HOH:O	2.42	0.50
1:A:145:ILE:HB	1:A:146:PRO:HD3	1.94	0.50
1:C:52:SER:N	3:C:516:HOH:O	2.44	0.50
1:B:230:ALA:HB1	1:B:276:ALA:HB2	1.93	0.50
1:D:59:LEU:HG	1:D:64:ALA:HB2	1.94	0.49
1:E:182:SER:HA	1:E:308:GLN:HB2	1.94	0.49
1:B:182:SER:OG	1:B:308:GLN:HB2	2.13	0.49
1:F:121:ILE:HG22	1:F:123:LEU:HG	1.93	0.49
1:E:256:PRO:HD2	3:E:674:HOH:O	2.11	0.49
1:C:21:ARG:NH2	3:C:517:HOH:O	2.45	0.49
1:D:145:ILE:HB	1:D:146:PRO:HD3	1.95	0.49
1:F:65:ASP:OD2	1:F:67:PRO:HD2	2.12	0.49
1:A:21:ARG:HD3	3:A:530:HOH:O	2.12	0.48
1:D:66:GLU:OE2	3:D:502:HOH:O	2.20	0.48
1:A:269:ARG:HA	1:A:273:LEU:O	2.13	0.48
1:F:1:MET:HA	1:F:1:MET:CE	2.42	0.48
1:C:53:ARG:HD2	1:C:53:ARG:HA	1.72	0.48
1:B:255:GLU:HG2	1:B:283:PRO:HB3	1.95	0.48
1:B:267:GLU:OE1	1:B:268:TRP:CD1	2.65	0.48
1:E:39:GLU:N	1:E:39:GLU:OE1	2.44	0.48
1:B:229:LEU:O	1:B:233:ILE:HG23	2.14	0.47
1:B:103:ILE:HD11	1:B:311:LEU:HD22	1.97	0.47
1:B:145:ILE:HB	1:B:146:PRO:HD3	1.95	0.47
1:D:80:ARG:HG2	1:D:85:ILE:HD11	1.94	0.47
1:E:230:ALA:HB1	1:E:276:ALA:HB2	1.96	0.47
1:F:115:LEU:HD13	1:F:130:LEU:HD11	1.97	0.47
1:F:5:THR:HG22	1:F:322:ILE:HD11	1.97	0.47
1:A:239:LEU:HD23	1:E:246:THR:HG21	1.96	0.47
1:C:323:GLU:OE1	3:C:501:HOH:O	2.20	0.47
1:B:39:GLU:OE1	1:B:39:GLU:N	2.45	0.47
1:C:269:ARG:HA	1:C:273:LEU:O	2.15	0.46
1:D:85:ILE:HG12	1:D:121:ILE:CD1	2.43	0.46
1:F:50:LYS:HD3	1:F:51:HIS:CE1	2.50	0.46
1:B:80:ARG:HD3	1:B:87:TRP:O	2.16	0.46
1:C:97:PHE:CE2	1:C:105:SER:HB3	2.51	0.46
1:F:78:ARG:HA	1:F:78:ARG:NE	2.31	0.46
1:E:92:ILE:N	1:E:92:ILE:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ILE:HG22	1:E:86:SER:H	1.79	0.46
1:F:233:ILE:HD11	1:F:276:ALA:HB3	1.98	0.46
1:E:182:SER:CA	1:E:308:GLN:HB2	2.46	0.46
1:C:230:ALA:CB	1:C:276:ALA:HB2	2.46	0.46
1:A:39:GLU:OE1	1:A:39:GLU:N	2.49	0.45
1:F:230:ALA:CB	1:F:276:ALA:HB2	2.46	0.45
1:A:66:GLU:HA	1:A:66:GLU:OE1	2.16	0.45
1:D:181:LEU:O	1:D:184:GLN:OE1	2.33	0.45
1:E:185:HIS:O	1:E:186:LYS:HE2	2.15	0.45
3:C:515:HOH:O	1:D:201:PRO:HG3	2.16	0.45
1:E:219:ARG:HD3	3:E:508:HOH:O	2.15	0.45
1:B:292:GLU:HG3	3:B:564:HOH:O	2.16	0.45
1:D:97:PHE:HE2	1:D:105:SER:HB3	1.78	0.45
1:B:-1:HIS:NE2	1:B:51:HIS:CB	2.79	0.45
1:E:269:ARG:HA	1:E:273:LEU:O	2.17	0.44
1:C:145:ILE:O	1:C:318:SER:HB2	2.18	0.44
1:D:103:ILE:HD11	1:D:311:LEU:HD12	2.00	0.44
1:E:48:PHE:CD1	1:E:89:ALA:HB2	2.52	0.44
1:F:185:HIS:HE1	1:F:187:PRO:HA	1.81	0.44
1:C:80:ARG:HD3	1:C:87:TRP:O	2.17	0.44
1:B:-1:HIS:CE1	1:B:51:HIS:HB2	2.52	0.44
1:E:9:HIS:HB3	1:E:37:LEU:O	2.17	0.44
1:D:230:ALA:CB	1:D:276:ALA:HB2	2.47	0.44
1:A:66:GLU:HB3	1:A:67:PRO:HD3	2.00	0.43
1:E:181:LEU:HB2	1:E:184:GLN:OE1	2.18	0.43
1:F:121:ILE:O	1:F:121:ILE:CG2	2.66	0.43
1:F:1:MET:HA	1:F:1:MET:HE2	2.00	0.43
1:A:97:PHE:CE2	1:A:105:SER:HB3	2.52	0.43
1:F:181:LEU:HD13	1:F:257:VAL:HB	2.00	0.43
1:B:145:ILE:HA	1:B:145:ILE:HD13	1.87	0.43
1:D:48:PHE:CZ	1:D:121:ILE:HD12	2.53	0.43
1:D:186:LYS:HB2	1:D:186:LYS:HE2	1.59	0.43
3:A:708:HOH:O	1:E:250:PRO:HG3	2.18	0.43
1:A:216:ILE:HD13	1:A:232:MET:CE	2.49	0.43
1:A:255:GLU:HG2	1:A:283:PRO:HB3	2.01	0.43
1:B:192:GLN:HG2	3:B:506:HOH:O	2.17	0.43
1:D:226:PHE:CE1	1:D:290:PRO:HD3	2.54	0.43
1:B:242:ALA:HB1	1:F:242:ALA:HB1	2.00	0.43
1:E:50:LYS:O	1:E:52:SER:N	2.52	0.43
1:B:168:PRO:HB2	1:B:170:GLU:OE1	2.19	0.42
1:C:3:GLN:HB2	1:C:47:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:PRO:HB2	1:D:101:ALA:HB2	2.01	0.42
1:B:159:GLU:HG3	3:B:668:HOH:O	2.17	0.42
1:F:184:GLN:O	1:F:185:HIS:HB3	2.18	0.42
1:A:50:LYS:HA	3:A:503:HOH:O	2.19	0.42
1:B:267:GLU:HG3	3:B:504:HOH:O	2.15	0.42
1:E:71:ARG:NH2	1:E:137:GLY:O	2.42	0.42
1:A:230:ALA:HB1	1:A:276:ALA:HB2	2.01	0.42
1:A:48:PHE:CZ	1:A:121:ILE:HD12	2.55	0.42
1:C:97:PHE:N	1:C:97:PHE:CD1	2.86	0.42
1:D:97:PHE:CD1	1:D:97:PHE:N	2.87	0.42
1:E:24:VAL:HG12	1:E:78:ARG:HH22	1.85	0.42
1:B:170:GLU:H	1:B:170:GLU:CD	2.23	0.42
1:A:51:HIS:HB2	3:A:607:HOH:O	2.20	0.41
1:B:7:ILE:HG23	1:B:322:ILE:HD13	2.02	0.41
1:D:9:HIS:HB3	1:D:37:LEU:O	2.20	0.41
1:F:226:PHE:CE1	1:F:290:PRO:HD3	2.55	0.41
1:B:252:PHE:HB3	1:F:263:LYS:HE2	2.02	0.41
1:F:85:ILE:HG22	1:F:86:SER:N	2.35	0.41
1:A:295:GLU:HG2	3:A:532:HOH:O	2.19	0.41
1:C:128:ARG:HD2	3:C:503:HOH:O	2.18	0.41
1:C:51:HIS:HB2	3:C:525:HOH:O	2.21	0.41
1:F:82:PHE:HE2	1:F:125:LEU:HD11	1.85	0.41
1:B:259:LEU:HA	1:B:259:LEU:HD23	1.85	0.41
1:B:-1:HIS:CE1	1:B:51:HIS:CD2	3.08	0.41
1:C:39:GLU:OE1	1:C:313:ALA:HA	2.21	0.41
1:E:178:ILE:O	1:E:310:VAL:HA	2.20	0.41
1:B:21:ARG:HG2	1:B:21:ARG:O	2.18	0.41
1:F:66:GLU:N	1:F:67:PRO:CD	2.84	0.41
1:F:9:HIS:HB3	1:F:37:LEU:O	2.20	0.41
1:E:26:ARG:HD3	1:E:135:ARG:O	2.21	0.41
1:A:103:ILE:O	3:A:502:HOH:O	2.22	0.41
1:A:255:GLU:OE1	3:A:501:HOH:O	2.21	0.41
1:A:295:GLU:OE2	1:A:312:LYS:NZ	2.25	0.41
1:C:1:MET:SD	1:C:1:MET:N	2.93	0.41
1:B:83:ALA:HB2	1:B:123:LEU:HD11	2.03	0.41
1:B:98:PRO:HG2	1:B:311:LEU:HD21	2.02	0.41
1:D:3:GLN:HA	1:D:46:VAL:O	2.21	0.41
1:E:57:LEU:HD11	1:E:59:LEU:CD2	2.50	0.41
1:F:85:ILE:HG22	1:F:87:TRP:H	1.86	0.41
1:E:57:LEU:C	1:E:58:ILE:HD13	2.42	0.40
1:F:42:VAL:HG22	1:F:95:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:PRO:HB2	1:F:170:GLU:OE2	2.21	0.40
1:A:160:ASP:OD2	1:C:160:ASP:OD2	2.39	0.40
1:C:226:PHE:CE1	1:C:290:PRO:HD3	2.55	0.40
1:C:78:ARG:HG3	3:C:689:HOH:O	2.20	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	321/330 (97%)	317 (99%)	4 (1%)	0	100	100
1	B	325/330 (98%)	316 (97%)	8 (2%)	1 (0%)	41	30
1	C	325/330 (98%)	320 (98%)	5 (2%)	0	100	100
1	D	323/330 (98%)	312 (97%)	10 (3%)	1 (0%)	41	30
1	E	319/330 (97%)	307 (96%)	12 (4%)	0	100	100
1	F	325/330 (98%)	316 (97%)	7 (2%)	2 (1%)	25	14
All	All	1938/1980 (98%)	1888 (97%)	46 (2%)	4 (0%)	47	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	182	SER
1	B	-1	HIS
1	D	82	PHE
1	F	308	GLN



### 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	262/268 (98%)	260 (99%)	2 (1%)	81	80
1	B	265/268 (99%)	261 (98%)	4 (2%)	65	60
1	C	265/268 (99%)	264 (100%)	1 (0%)	91	90
1	D	264/268 (98%)	259 (98%)	5 (2%)	57	50
1	E	261/268 (97%)	257 (98%)	4 (2%)	65	60
1	F	266/268 (99%)	262 (98%)	4 (2%)	65	60
All	All	1583/1608 (98%)	1563 (99%)	20 (1%)	69	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	TYR
1	A	317	ASP
1	B	17	TYR
1	B	54	GLU
1	B	71	ARG
1	B	185	HIS
1	C	17	TYR
1	D	-1	HIS
1	D	17	TYR
1	D	82	PHE
1	D	183	THR
1	D	317	ASP
1	E	51	HIS
1	E	185	HIS
1	E	259	LEU
1	E	317	ASP
1	F	17	TYR
1	F	71	ARG
1	F	184	GLN
1	F	317	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	HIS
1	C	184	GLN
1	D	74	HIS
1	E	308	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	DP6	D	401	-	11,17,17	1.12	1 (9%)	14,26,26	0.83	0
2	DP6	F	401	-	11,17,17	1.04	1 (9%)	14,26,26	0.87	0
2	DP6	E	401	-	11,17,17	0.82	0	14,26,26	0.94	0
2	DP6	B	401	-	11,17,17	1.29	1 (9%)	14,26,26	0.79	1 (7%)
2	DP6	A	401	-	11,17,17	1.01	1 (9%)	14,26,26	0.70	0
2	DP6	C	401	-	11,17,17	1.07	0	14,26,26	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DP6	D	401	-	-	4/17/19/19	-
2	DP6	F	401	-	-	3/17/19/19	-
2	DP6	E	401	-	-	5/17/19/19	-
2	DP6	B	401	-	-	5/17/19/19	-
2	DP6	A	401	-	-	4/17/19/19	-
2	DP6	C	401	-	-	3/17/19/19	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	DP6	O3A-C3	-3.10	1.40	1.44
2	D	401	DP6	O3A-C3	-2.82	1.40	1.44
2	A	401	DP6	O3A-C3	-2.16	1.41	1.44
2	F	401	DP6	C2-C3	-2.08	1.51	1.55

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	DP6	O2B-PB-O6	2.08	111.62	104.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	DP6	C3A-C3-C4-C5
2	D	401	DP6	C2-C3-C4-C5
2	E	401	DP6	C3A-C3-C4-C5
2	E	401	DP6	C2-C3-C4-C5
2	B	401	DP6	C5-O5-PA-O1A
2	B	401	DP6	C3A-C3-C4-C5
2	B	401	DP6	C2-C3-C4-C5
2	A	401	DP6	C5-O5-PA-O1A
2	A	401	DP6	C3A-C3-C4-C5
2	A	401	DP6	C2-C3-C4-C5
2	C	401	DP6	C3A-C3-C4-C5
2	C	401	DP6	C2-C3-C4-C5
2	F	401	DP6	C3A-C3-C4-C5

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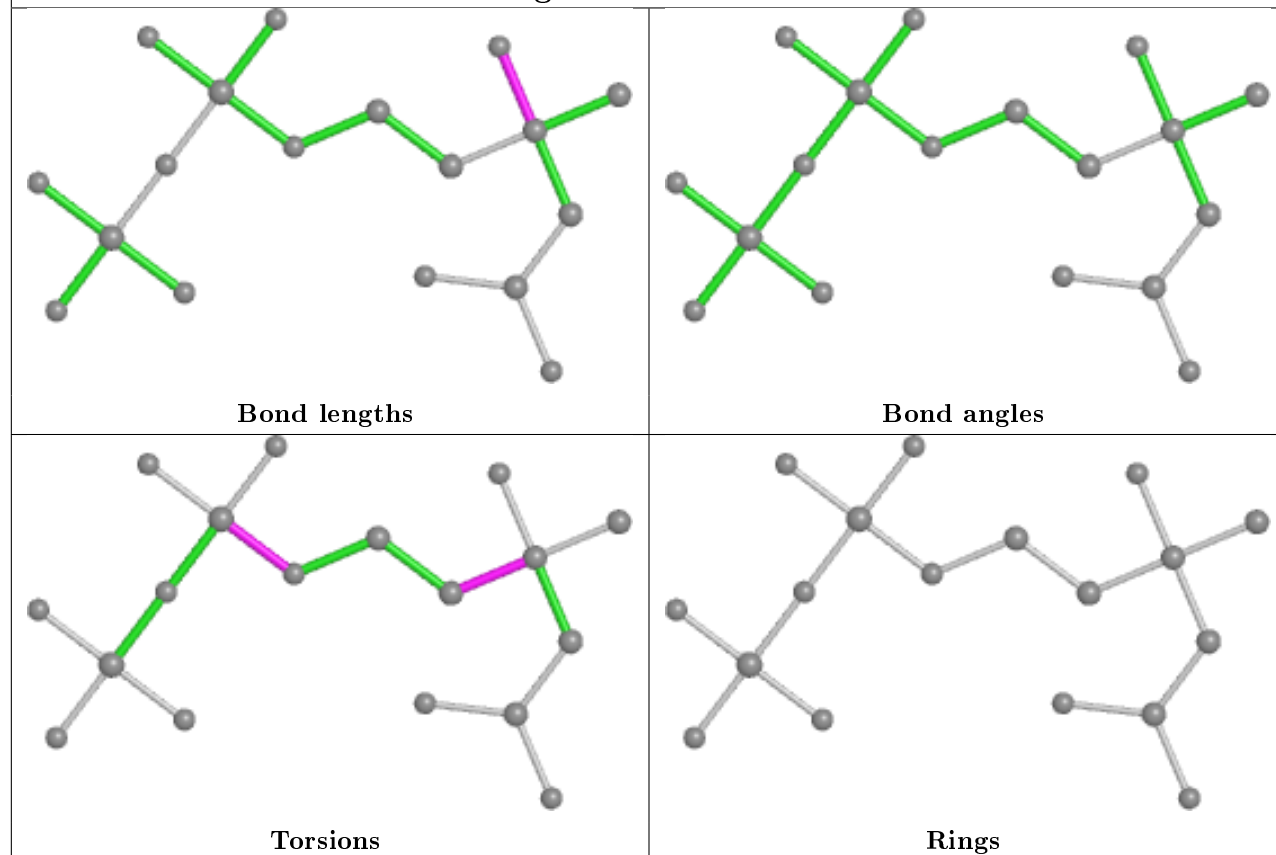
Mol	Chain	Res	Type	Atoms
2	F	401	DP6	C2-C3-C4-C5
2	F	401	DP6	O3A-C3-C4-C5
2	E	401	DP6	O3A-C3-C4-C5
2	B	401	DP6	C5-O5-PA-O6
2	E	401	DP6	PA-O6-PB-O1B
2	D	401	DP6	O3A-C3-C4-C5
2	E	401	DP6	C5-O5-PA-O6
2	B	401	DP6	O3A-C3-C4-C5
2	A	401	DP6	C5-O5-PA-O6
2	C	401	DP6	O3A-C3-C4-C5
2	D	401	DP6	C5-O5-PA-O1A

There are no ring outliers.

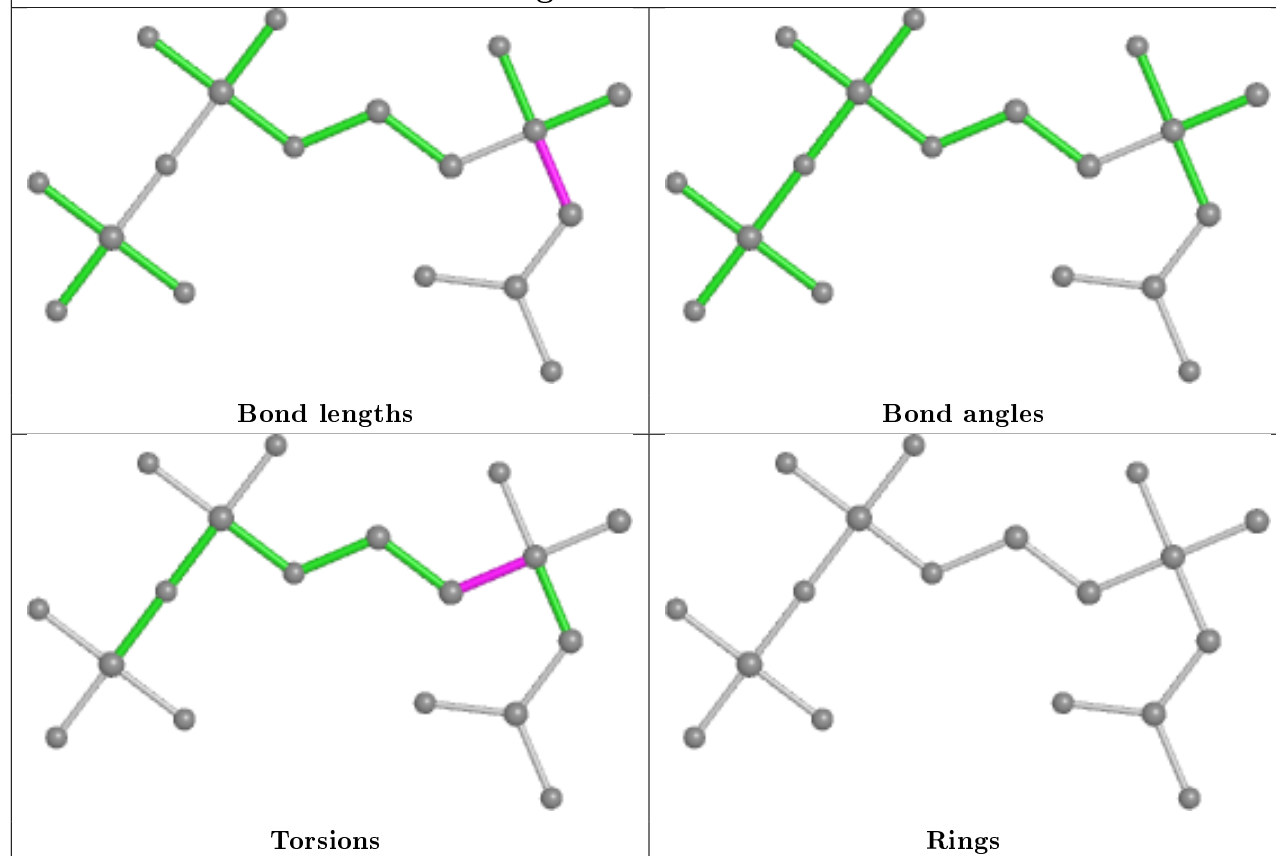
No monomer is involved in short contacts.

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.

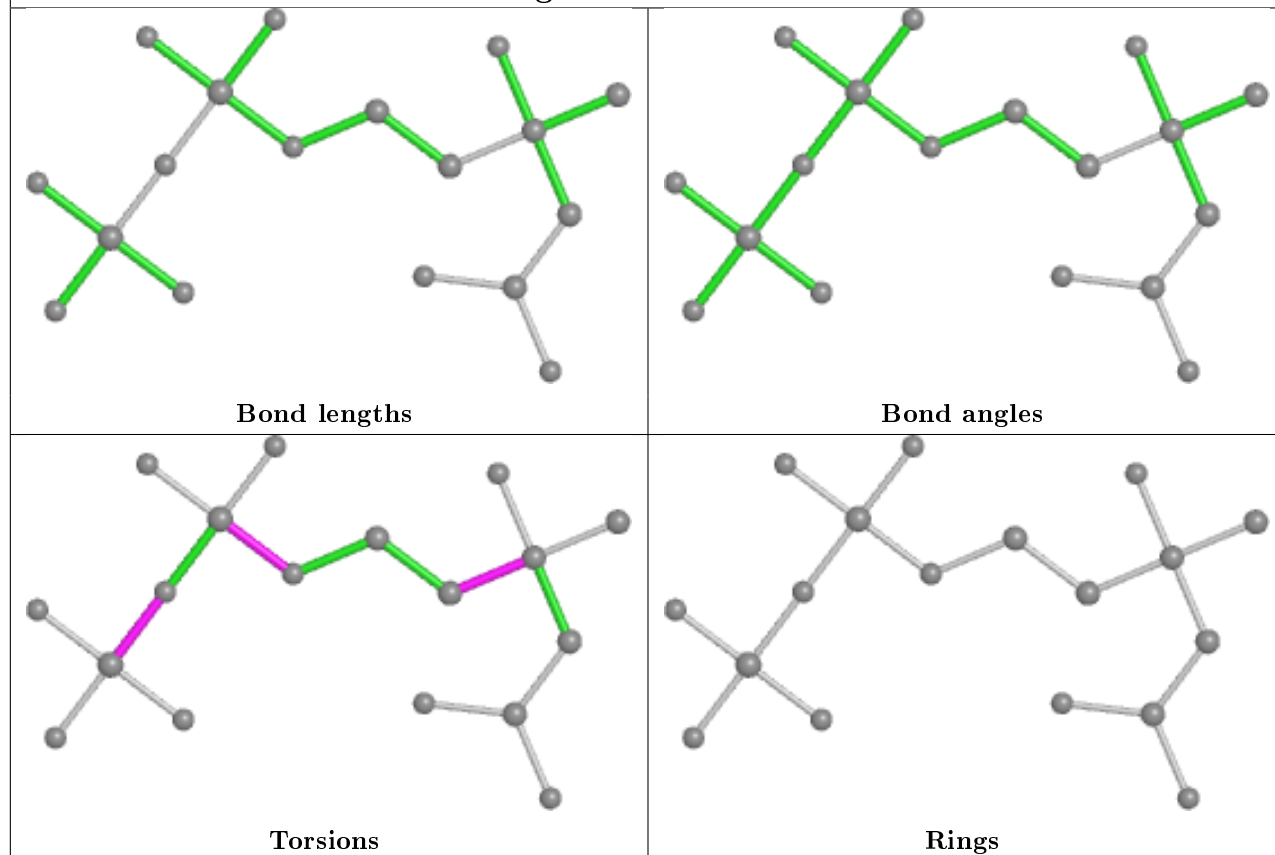
## Ligand DP6 D 401



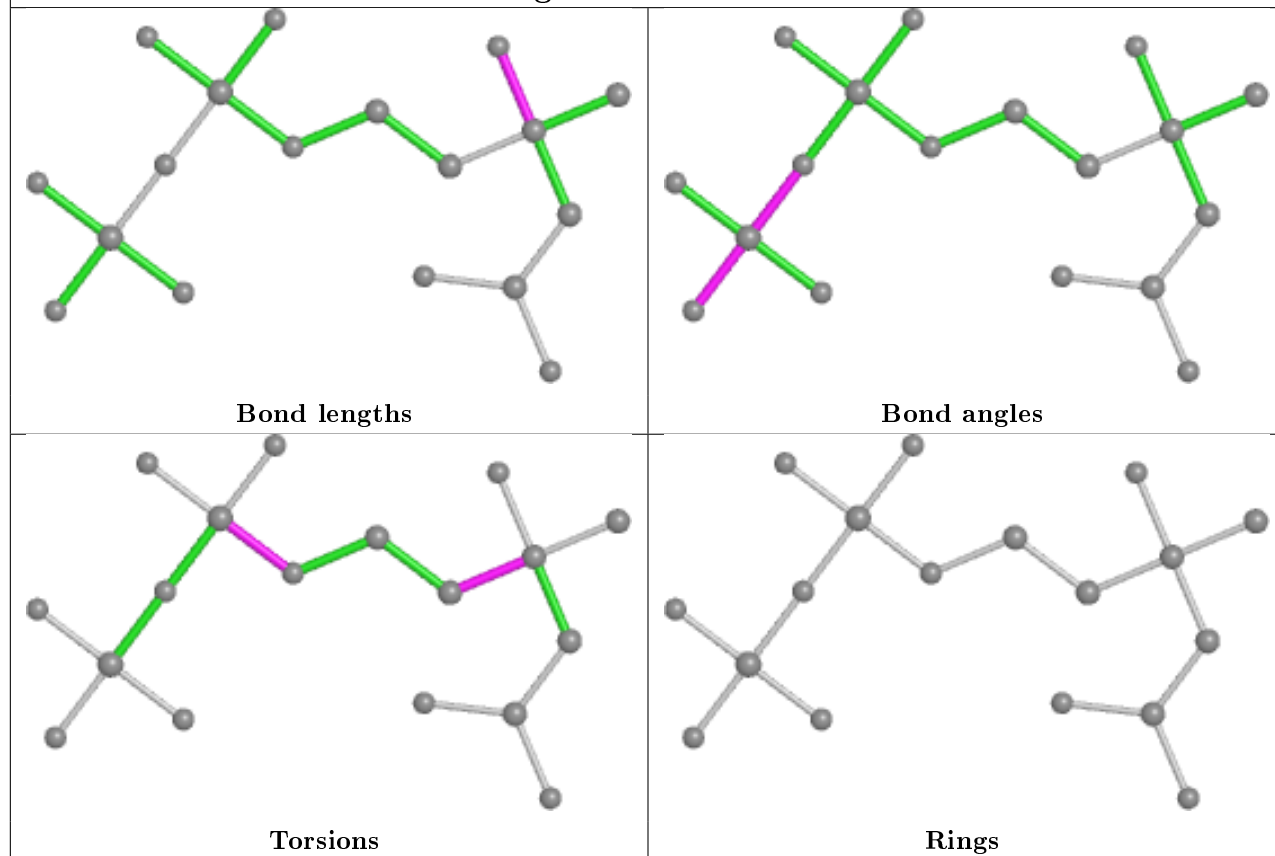
## Ligand DP6 F 401



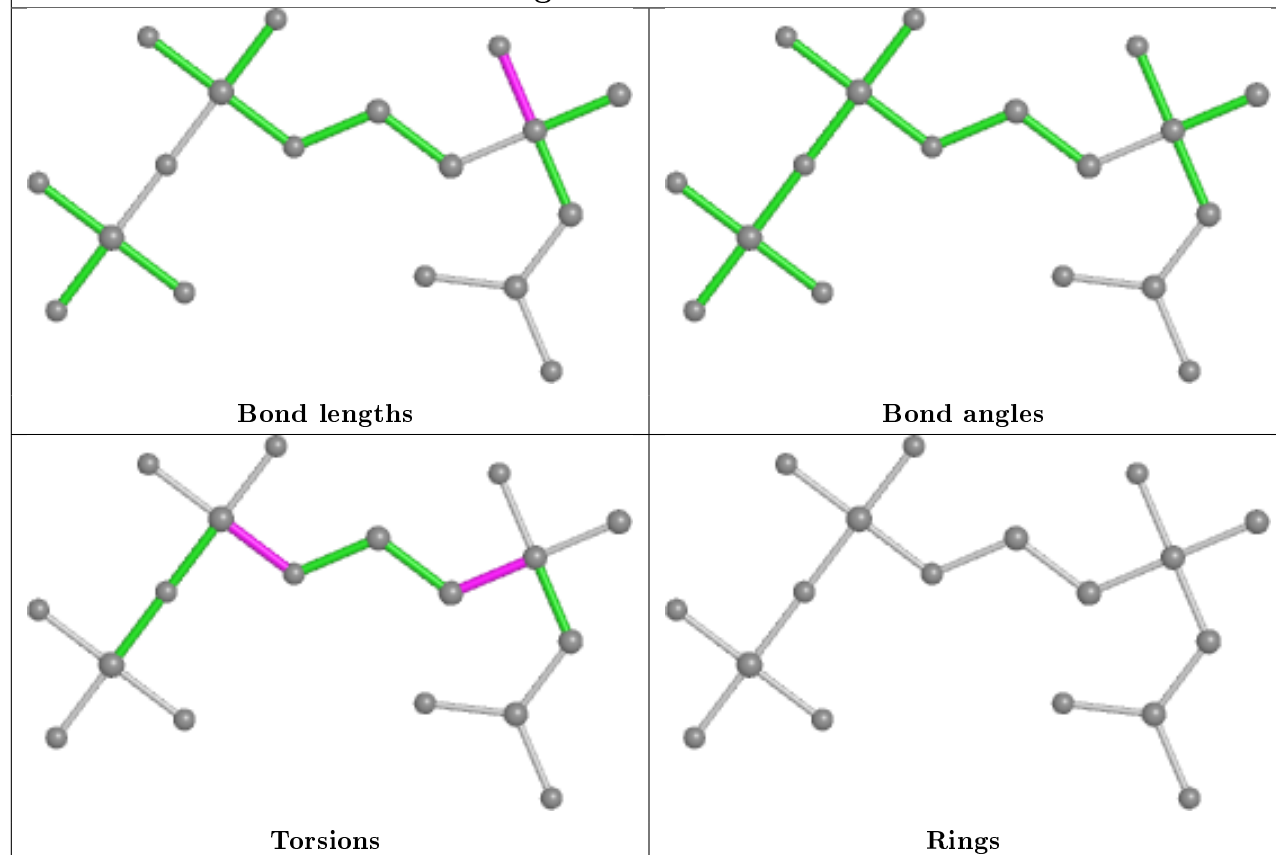
## Ligand DP6 E 401



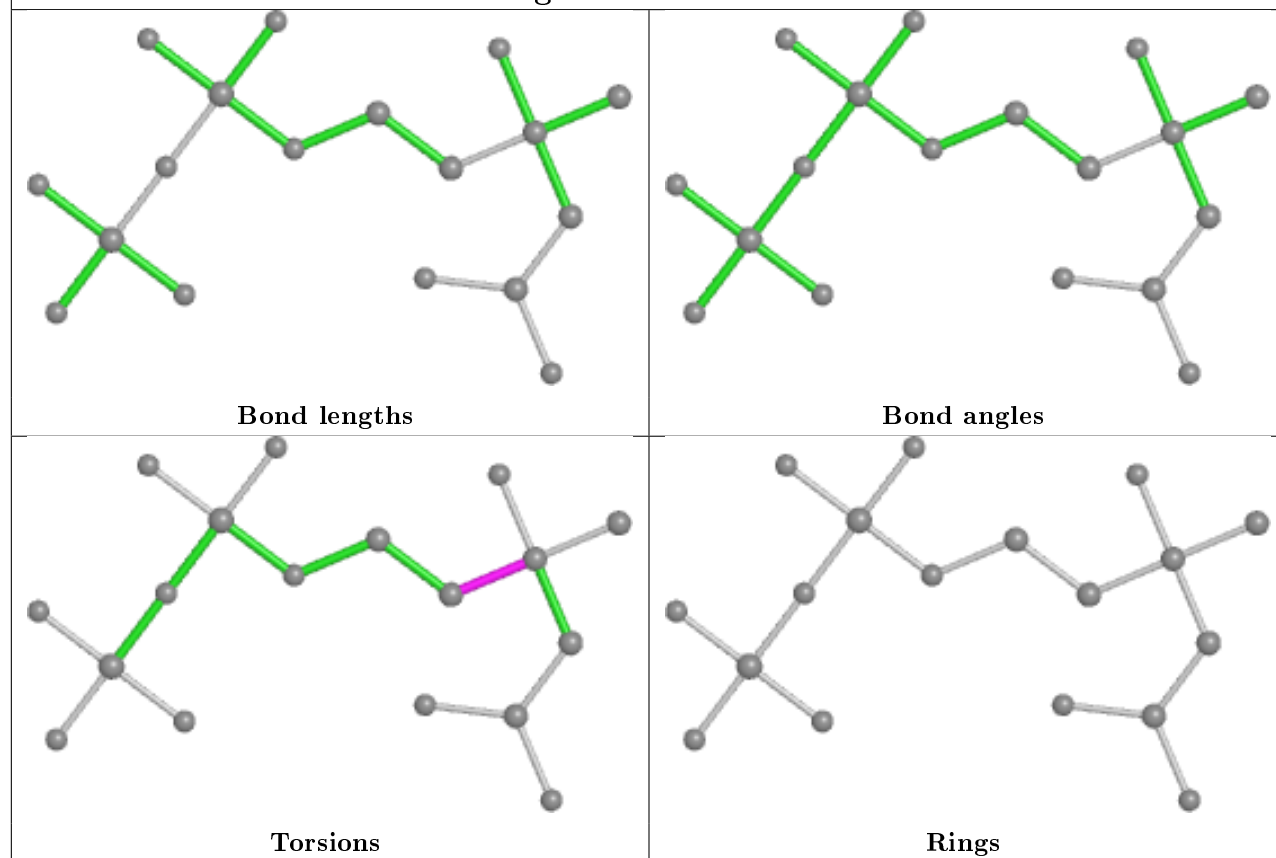
## Ligand DP6 B 401



## Ligand DP6 A 401



## Ligand DP6 C 401



## 5.7 Other polymers

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/330 (97%)	-0.00	11 (3%) 45 55	11, 20, 42, 61	0
1	B	327/330 (99%)	0.09	13 (3%) 38 48	10, 19, 40, 65	0
1	C	327/330 (99%)	0.09	9 (2%) 53 62	10, 18, 41, 72	0
1	D	325/330 (98%)	0.02	12 (3%) 41 51	11, 21, 44, 68	0
1	E	321/330 (97%)	0.42	32 (9%) 7 11	11, 23, 52, 87	0
1	F	327/330 (99%)	0.05	11 (3%) 45 55	11, 22, 41, 68	0
All	All	1950/1980 (98%)	0.11	88 (4%) 33 43	10, 21, 46, 87	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	51	HIS	9.5
1	E	87	TRP	7.2
1	E	50	LYS	6.7
1	D	51	HIS	5.6
1	E	53	ARG	5.0
1	D	183	THR	5.0
1	C	51	HIS	4.8
1	E	69	LEU	4.8
1	C	53	ARG	4.8
1	D	53	ARG	4.6
1	F	51	HIS	4.6
1	E	54	GLU	4.6
1	E	52	SER	4.1
1	A	53	ARG	4.1
1	B	-1	HIS	4.0
1	F	183	THR	3.9
1	E	85	ILE	3.9
1	F	185	HIS	3.9
1	F	53	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	-1	HIS	3.7
1	E	82	PHE	3.7
1	B	184	GLN	3.7
1	D	82	PHE	3.7
1	B	183	THR	3.6
1	A	51	HIS	3.6
1	E	86	SER	3.6
1	E	56	THR	3.5
1	C	0	GLY	3.5
1	E	84	GLY	3.5
1	D	-2	SER	3.4
1	E	49	GLU	3.4
1	B	51	HIS	3.4
1	E	61	GLY	3.3
1	B	-2	SER	3.3
1	C	87	TRP	3.3
1	A	103	ILE	3.2
1	F	182	SER	3.2
1	C	54	GLU	3.2
1	F	87	TRP	3.2
1	F	184	GLN	3.2
1	E	90	HIS	3.2
1	B	-3	GLY	3.2
1	E	57	LEU	3.0
1	D	103	ILE	3.0
1	A	102	GLY	2.9
1	D	100	GLY	2.9
1	E	55	ASP	2.9
1	F	50	LYS	2.9
1	D	98	PRO	2.8
1	A	104	ALA	2.8
1	B	185	HIS	2.7
1	C	184	GLN	2.7
1	E	183	THR	2.7
1	D	52	SER	2.7
1	A	82	PHE	2.6
1	E	48	PHE	2.6
1	B	267	GLU	2.6
1	A	100	GLY	2.6
1	E	120	ALA	2.6
1	E	64	ALA	2.5
1	E	76	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	53	ARG	2.5
1	E	63	LEU	2.5
1	E	185	HIS	2.4
1	B	182	SER	2.4
1	B	323	GLU	2.3
1	E	122	GLY	2.3
1	E	66	GLU	2.3
1	C	82	PHE	2.3
1	D	54	GLU	2.3
1	E	117	ALA	2.2
1	B	65	ASP	2.2
1	C	74	HIS	2.2
1	E	124	HIS	2.2
1	A	184	GLN	2.2
1	C	52	SER	2.2
1	B	103	ILE	2.2
1	F	54	GLU	2.2
1	A	101	ALA	2.2
1	E	59	LEU	2.1
1	D	185	HIS	2.1
1	E	92	ILE	2.1
1	F	52	SER	2.1
1	A	54	GLU	2.1
1	A	52	SER	2.0
1	E	65	ASP	2.0
1	E	88	HIS	2.0
1	F	66	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 [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,

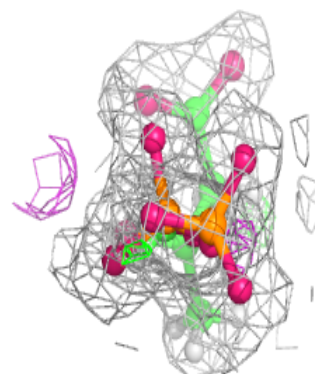
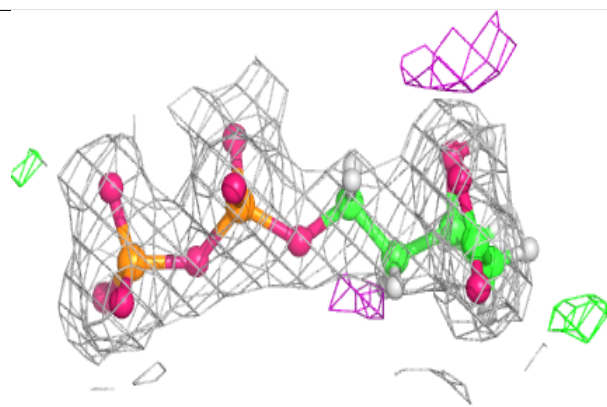
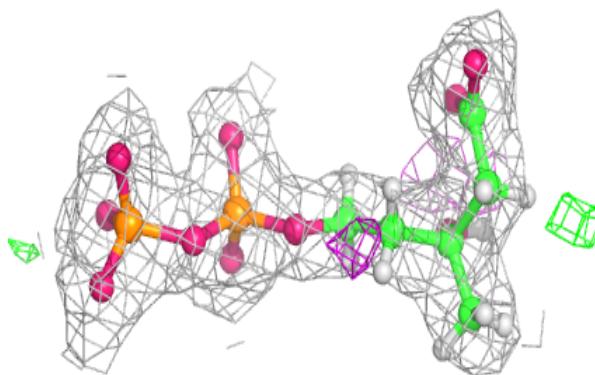
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DP6	D	401	18/18	0.99	0.08	14,18,21,23	0
2	DP6	F	401	18/18	0.99	0.08	13,20,28,28	0
2	DP6	E	401	18/18	0.99	0.09	14,20,27,27	0
2	DP6	B	401	18/18	0.99	0.09	9,17,21,24	0
2	DP6	A	401	18/18	0.99	0.09	13,22,27,28	0
2	DP6	C	401	18/18	0.99	0.08	11,17,22,22	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.

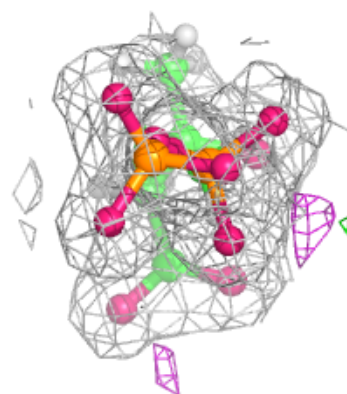
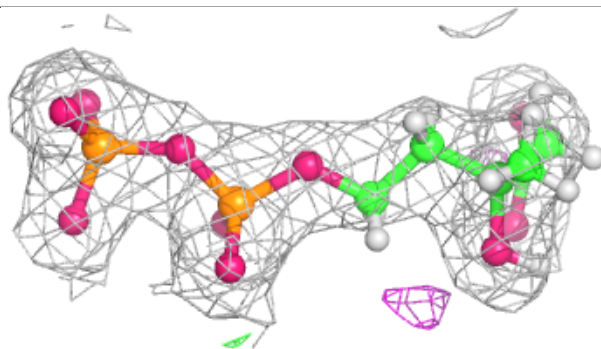
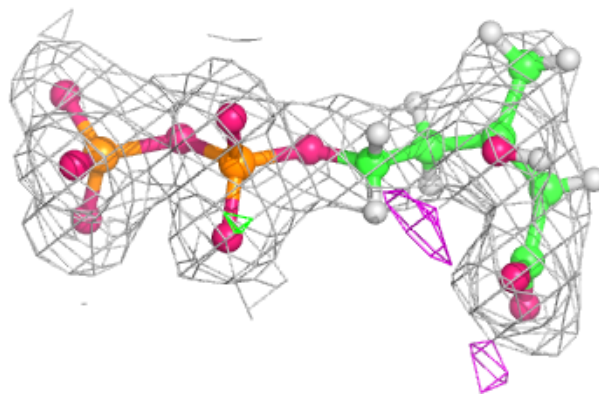
**Electron density around DP6 D 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

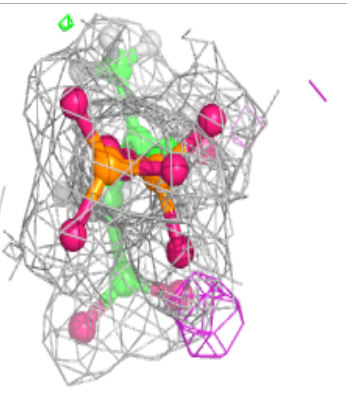
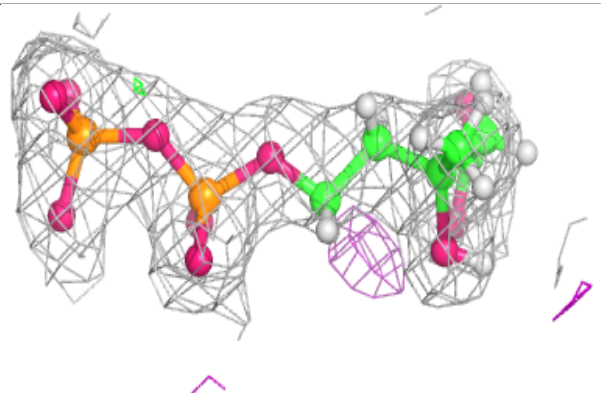
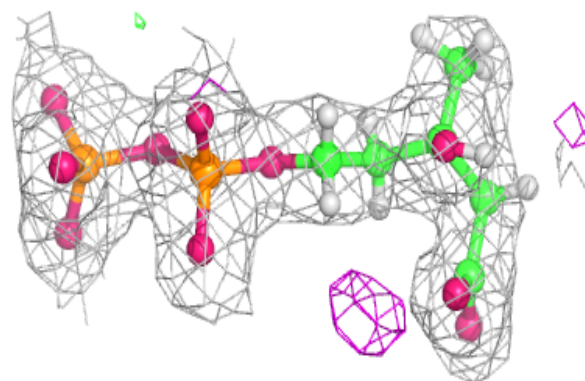


**Electron density around DP6 F 401:**

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

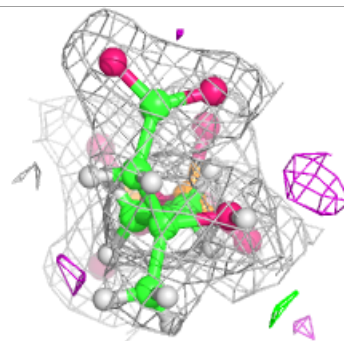
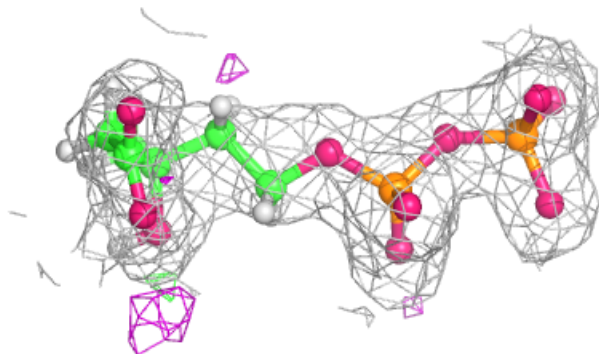
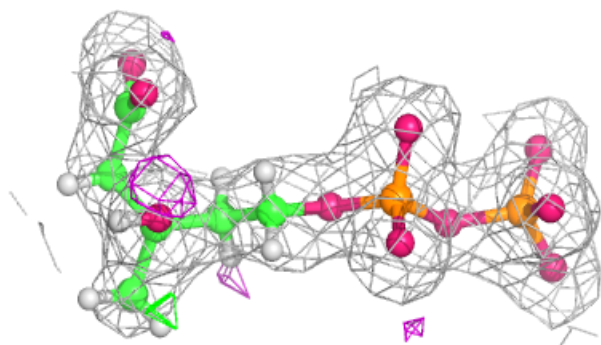
**Electron density around DP6 E 401:**

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

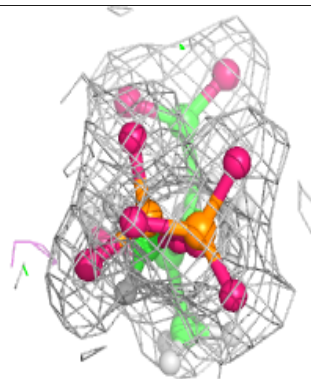
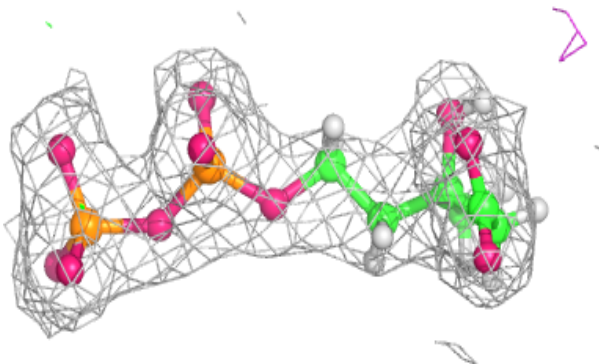
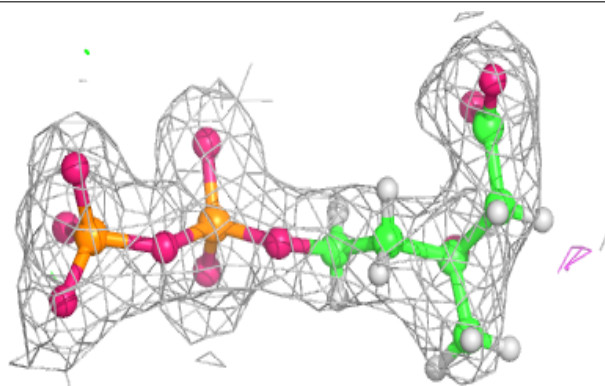


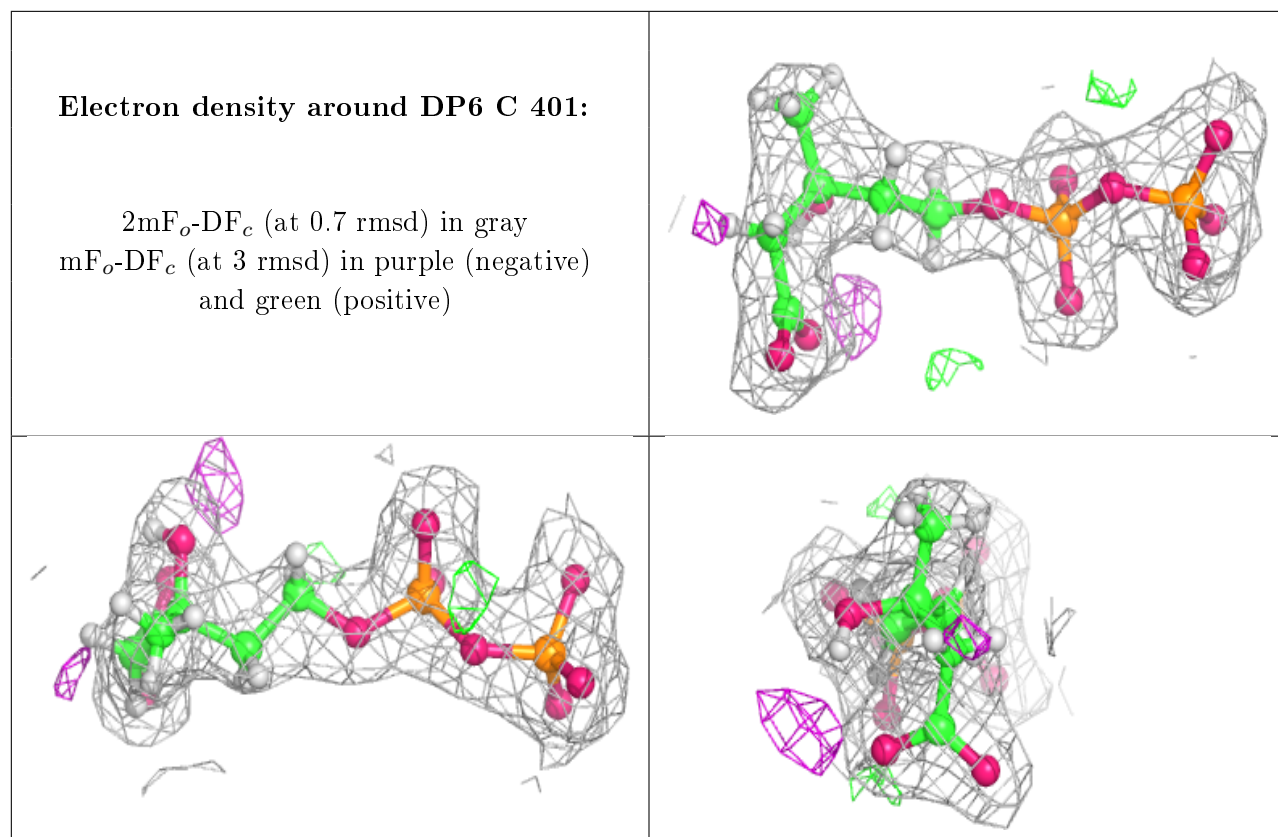
**Electron density around DP6 B 401:**

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

**Electron density around DP6 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.