



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 11:25 pm BST

PDB ID : 3MAU  
Title : Crystal structure of StSPL in complex with phosphoethanolamine  
Authors : Bourquin, F.; Grutter, M.G.; Capitani, G.  
Deposited on : 2010-03-24  
Resolution : 2.90 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 : 2.11  
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) : 2.11

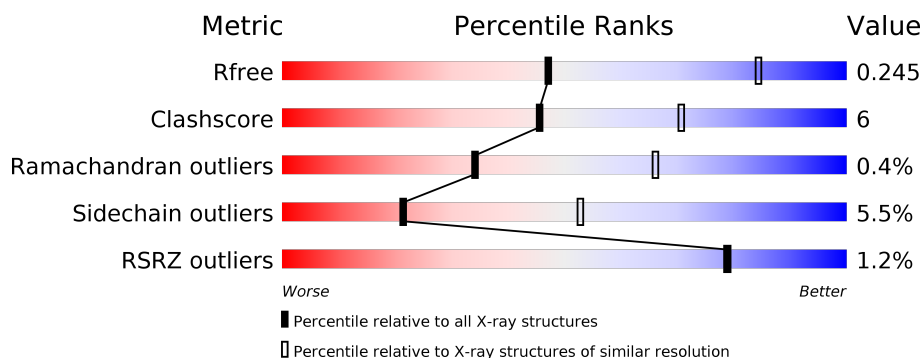
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	514	<div> <div>72%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>
1	B	514	<div> <div>2%</div> <div>71%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>
1	C	514	<div> <div>2%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>12%</div> </div>
1	D	514	<div> <div>2%</div> <div>72%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13842 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 sphingosine-1-phosphate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	1	0
			3429	2195	600	621	13			
1	B	451	Total	C	N	O	S	0	2	0
			3429	2195	602	619	13			
1	C	452	Total	C	N	O	S	0	0	0
			3423	2191	599	620	13			
1	D	452	Total	C	N	O	S	0	0	0
			3423	2191	599	620	13			

There are 36 discrepancies between the modelled and reference sequences:

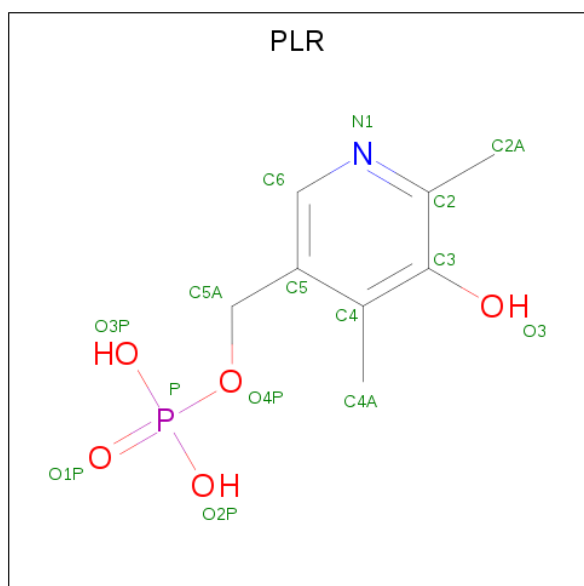
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q67PY4
A	1	PRO	-	EXPRESSION TAG	UNP Q67PY4
A	311	ALA	LYS	ENGINEERED MUTATION	UNP Q67PY4
A	508	HIS	-	EXPRESSION TAG	UNP Q67PY4
A	509	HIS	-	EXPRESSION TAG	UNP Q67PY4
A	510	HIS	-	EXPRESSION TAG	UNP Q67PY4
A	511	HIS	-	EXPRESSION TAG	UNP Q67PY4
A	512	HIS	-	EXPRESSION TAG	UNP Q67PY4
A	513	HIS	-	EXPRESSION TAG	UNP Q67PY4
B	0	MET	-	EXPRESSION TAG	UNP Q67PY4
B	1	PRO	-	EXPRESSION TAG	UNP Q67PY4
B	311	ALA	LYS	ENGINEERED MUTATION	UNP Q67PY4
B	508	HIS	-	EXPRESSION TAG	UNP Q67PY4
B	509	HIS	-	EXPRESSION TAG	UNP Q67PY4
B	510	HIS	-	EXPRESSION TAG	UNP Q67PY4
B	511	HIS	-	EXPRESSION TAG	UNP Q67PY4
B	512	HIS	-	EXPRESSION TAG	UNP Q67PY4
B	513	HIS	-	EXPRESSION TAG	UNP Q67PY4
C	0	MET	-	EXPRESSION TAG	UNP Q67PY4
C	1	PRO	-	EXPRESSION TAG	UNP Q67PY4
C	311	ALA	LYS	ENGINEERED MUTATION	UNP Q67PY4

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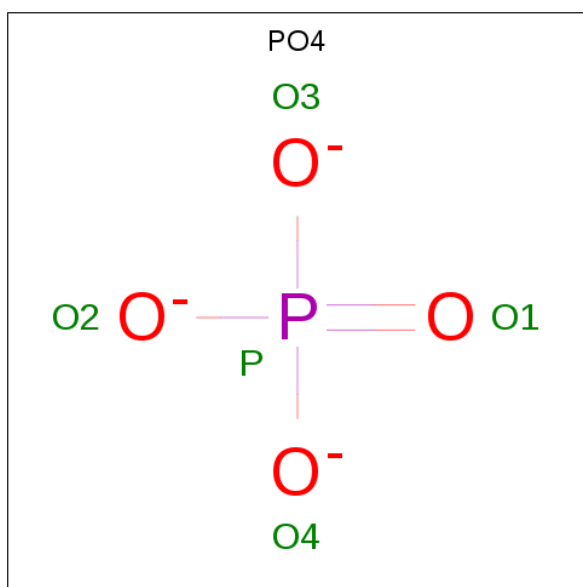
Chain	Residue	Modelled	Actual	Comment	Reference
C	508	HIS	-	EXPRESSION TAG	UNP Q67PY4
C	509	HIS	-	EXPRESSION TAG	UNP Q67PY4
C	510	HIS	-	EXPRESSION TAG	UNP Q67PY4
C	511	HIS	-	EXPRESSION TAG	UNP Q67PY4
C	512	HIS	-	EXPRESSION TAG	UNP Q67PY4
C	513	HIS	-	EXPRESSION TAG	UNP Q67PY4
D	0	MET	-	EXPRESSION TAG	UNP Q67PY4
D	1	PRO	-	EXPRESSION TAG	UNP Q67PY4
D	311	ALA	LYS	ENGINEERED MUTATION	UNP Q67PY4
D	508	HIS	-	EXPRESSION TAG	UNP Q67PY4
D	509	HIS	-	EXPRESSION TAG	UNP Q67PY4
D	510	HIS	-	EXPRESSION TAG	UNP Q67PY4
D	511	HIS	-	EXPRESSION TAG	UNP Q67PY4
D	512	HIS	-	EXPRESSION TAG	UNP Q67PY4
D	513	HIS	-	EXPRESSION TAG	UNP Q67PY4

- Molecule 2 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula: C<sub>8</sub>H<sub>12</sub>NO<sub>5</sub>P).



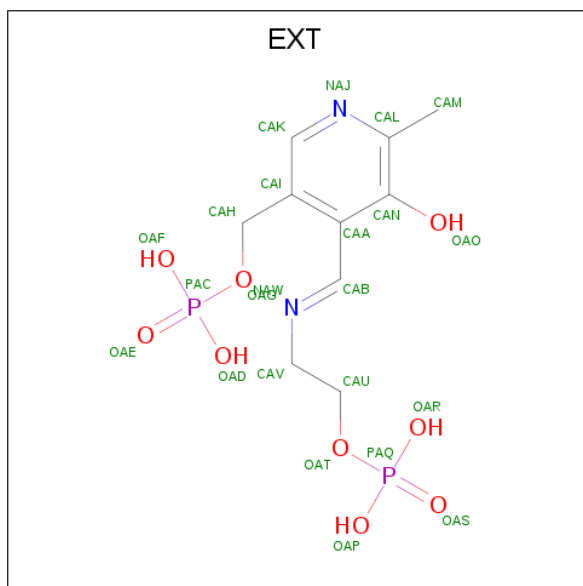
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is {5-hydroxy-6-methyl-4-[(E)-{[2-(phosphonooxy)ethyl]imino} methyl]pyridin-3-yl}methyl dihydrogen phosphate (three-letter code: EXT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>9</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	10	2	9	2		
4	C	1	Total	C	N	O	P	0	0
			23	10	2	9	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			23	10	2	9	2		

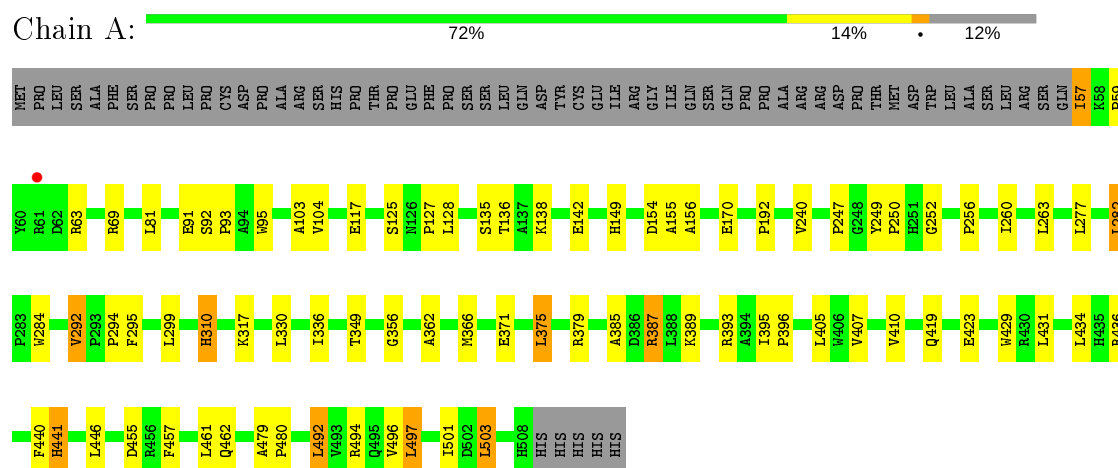
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	17	Total	O	0	0
			17	17		
5	C	10	Total	O	0	0
			10	10		
5	D	10	Total	O	0	0
			10	10		

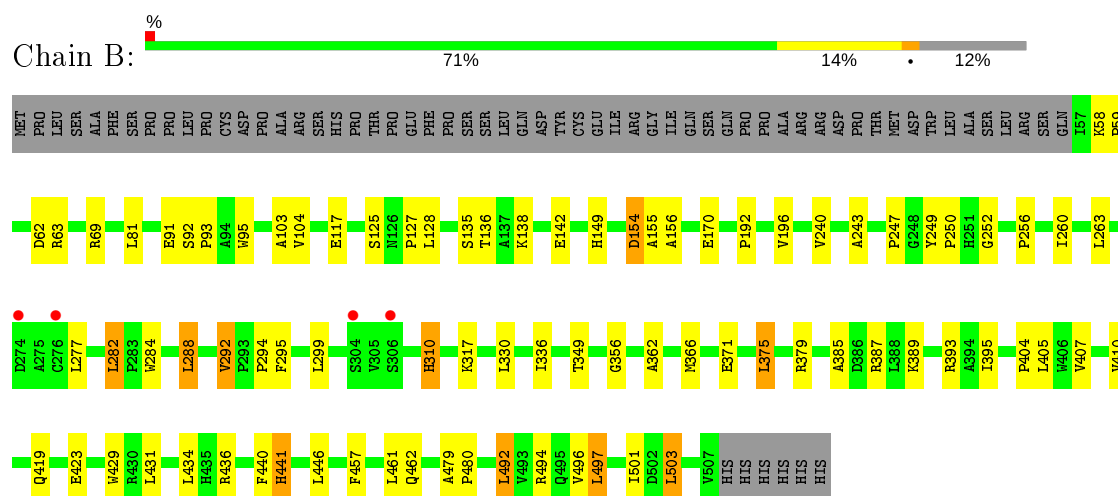
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

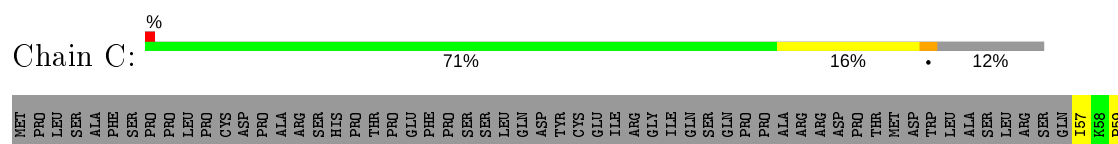
- Molecule 1: sphingosine-1-phosphate lyase

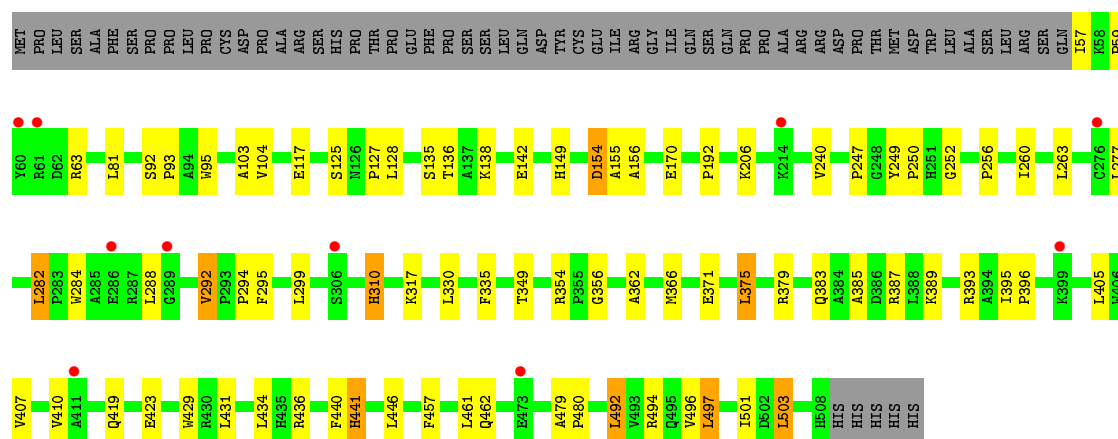


- Molecule 1: sphingosine-1-phosphate lyase



- Molecule 1: sphingosine-1-phosphate lyase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.36Å 243.45Å 280.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.90 29.89 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.89-2.90) 97.8 (29.89-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.4 _29	Depositor
R, $R_{free}$	0.229 , 0.252 0.222 , 0.245	Depositor DCC
$R_{free}$ test set	2421 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 12.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: PO4, EXT, PLR

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	0.30	0/3530	0.62	8/4824 (0.2%)
1	B	0.30	0/3532	0.71	9/4825 (0.2%)
1	C	0.29	0/3521	0.62	8/4812 (0.2%)
1	D	0.30	0/3521	0.61	8/4812 (0.2%)
All	All	0.30	0/14104	0.64	33/19273 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ARG	NE-CZ-NH1	-18.07	111.26	120.30
1	B	393	ARG	NE-CZ-NH2	17.57	129.08	120.30
1	D	387	ARG	NE-CZ-NH1	-13.26	113.67	120.30
1	C	387	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	A	387	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	D	387	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	C	379	ARG	NE-CZ-NH2	-12.54	114.03	120.30
1	A	379	ARG	NE-CZ-NH2	-12.33	114.14	120.30
1	C	387	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	A	387	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	B	387	ARG	NE-CZ-NH1	-12.02	114.29	120.30
1	A	379	ARG	NE-CZ-NH1	11.99	126.29	120.30
1	B	379	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	C	379	ARG	NE-CZ-NH1	11.89	126.25	120.30
1	D	379	ARG	NE-CZ-NH1	-11.63	114.49	120.30
1	B	387	ARG	NE-CZ-NH2	11.17	125.89	120.30
1	B	379	ARG	NE-CZ-NH2	10.96	125.78	120.30
1	D	379	ARG	NE-CZ-NH2	10.73	125.67	120.30
1	B	393	ARG	CD-NE-CZ	9.24	136.53	123.60
1	A	393	ARG	NE-CZ-NH2	-7.17	116.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	393	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	387	ARG	CD-NE-CZ	6.48	132.67	123.60
1	C	387	ARG	CD-NE-CZ	6.38	132.53	123.60
1	A	393	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	393	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	379	ARG	CD-NE-CZ	6.08	132.12	123.60
1	A	379	ARG	CD-NE-CZ	6.08	132.11	123.60
1	B	379	ARG	CD-NE-CZ	5.89	131.85	123.60
1	D	393	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	387	ARG	CD-NE-CZ	5.75	131.65	123.60
1	D	379	ARG	CD-NE-CZ	5.59	131.43	123.60
1	D	387	ARG	CD-NE-CZ	5.54	131.35	123.60
1	C	393	ARG	NE-CZ-NH1	5.46	123.03	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3429	0	3370	44	0
1	B	3429	0	3381	49	0
1	C	3423	0	3362	51	0
1	D	3423	0	3362	44	0
2	A	15	0	10	2	0
3	A	5	0	0	0	0
4	B	23	0	11	1	0
4	C	23	0	12	0	0
4	D	23	0	11	0	0
5	A	12	0	0	0	0
5	B	17	0	0	3	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
All	All	13842	0	13519	175	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 6.

All (175) 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:503:LEU:O	1:A:503:LEU:HD22	1.98	0.64
1:B:138:LYS:HE2	1:B:142:GLU:OE2	1.98	0.63
1:C:503:LEU:O	1:C:503:LEU:HD22	1.98	0.63
1:A:138:LYS:HE2	1:A:142:GLU:OE2	2.00	0.61
1:B:404:PRO:HG3	5:B:528:HOH:O	2.01	0.61
1:C:138:LYS:HE2	1:C:142:GLU:OE2	2.01	0.60
1:D:503:LEU:HD22	1:D:503:LEU:O	2.00	0.60
1:D:434:LEU:HD11	1:D:441:HIS:HB3	1.83	0.59
1:D:138:LYS:HE2	1:D:142:GLU:OE2	2.03	0.59
1:A:434:LEU:HD11	1:A:441:HIS:HB3	1.85	0.58
1:B:434:LEU:HD11	1:B:441:HIS:HB3	1.85	0.58
1:C:434:LEU:HD11	1:C:441:HIS:HB3	1.86	0.58
1:B:503:LEU:HD22	1:B:503:LEU:O	2.03	0.58
1:B:62:ASP:HB3	1:C:89:ALA:HB3	1.85	0.58
2:A:514:PLR:H4A1	2:A:514:PLR:O1P	2.04	0.58
1:B:479:ALA:HB3	1:B:480:PRO:HD3	1.86	0.58
1:C:479:ALA:HB3	1:C:480:PRO:HD3	1.85	0.58
1:D:362:ALA:O	1:D:366:MET:HG3	2.05	0.57
1:D:479:ALA:HB3	1:D:480:PRO:HD3	1.86	0.57
1:C:387:ARG:NH2	1:C:455:ASP:OD1	2.38	0.56
1:C:362:ALA:O	1:C:366:MET:HG3	2.05	0.56
1:D:294:PRO:O	1:D:299:LEU:HD11	2.05	0.56
1:B:362:ALA:O	1:B:366:MET:HG3	2.06	0.55
1:A:362:ALA:O	1:A:366:MET:HG3	2.07	0.55
1:A:294:PRO:O	1:A:299:LEU:HD11	2.07	0.55
1:C:294:PRO:O	1:C:299:LEU:HD11	2.07	0.54
1:C:95:TRP:CD2	1:C:104:VAL:HG21	2.43	0.54
1:A:387:ARG:NH2	1:A:455:ASP:OD1	2.40	0.54
1:A:479:ALA:HB3	1:A:480:PRO:HD3	1.90	0.53
1:A:497:LEU:HB3	1:B:336:ILE:HD13	1.90	0.53
1:C:127:PRO:HG3	1:C:136:THR:HG21	1.90	0.53
1:A:127:PRO:HG3	1:A:136:THR:HG21	1.89	0.52
1:D:256:PRO:O	1:D:260:ILE:HG13	2.10	0.52
1:A:497:LEU:O	1:A:501:ILE:HG13	2.10	0.51
1:B:294:PRO:O	1:B:299:LEU:HD11	2.10	0.51
1:A:170:GLU:OE2	1:A:349:THR:HB	2.10	0.51
1:D:125:SER:OG	1:D:356:GLY:HA3	2.10	0.51
1:A:95:TRP:CD2	1:A:104:VAL:HG21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:PRO:HG3	1:D:136:THR:HG21	1.91	0.51
1:D:95:TRP:CD2	1:D:104:VAL:HG21	2.45	0.51
1:C:256:PRO:O	1:C:260:ILE:HG13	2.12	0.50
1:C:91:GLU:OE2	1:D:135:SER:HB3	2.11	0.50
1:B:127:PRO:HG3	1:B:136:THR:HG21	1.92	0.50
1:A:256:PRO:O	1:A:260:ILE:HG13	2.11	0.50
1:B:441:HIS:C	1:B:441:HIS:ND1	2.64	0.50
1:D:282:LEU:HB3	1:D:295:PHE:CE2	2.46	0.50
1:B:170:GLU:OE2	1:B:349:THR:HB	2.11	0.50
1:A:336:ILE:HD13	1:B:497:LEU:HB3	1.94	0.50
1:A:154:ASP:C	1:A:156:ALA:H	2.14	0.50
1:A:117:GLU:HG2	1:B:81:LEU:HD13	1.95	0.49
1:B:95:TRP:CD2	1:B:104:VAL:HG21	2.47	0.49
1:C:154:ASP:C	1:C:156:ALA:H	2.15	0.49
1:C:282:LEU:HB3	1:C:295:PHE:CE2	2.48	0.49
1:D:284:TRP:CH2	1:D:371:GLU:HG2	2.47	0.49
1:A:249:TYR:N	1:A:250:PRO:CD	2.76	0.49
1:B:125:SER:OG	1:B:356:GLY:HA3	2.11	0.49
1:C:441:HIS:C	1:C:441:HIS:ND1	2.66	0.49
1:C:497:LEU:O	1:C:501:ILE:HG13	2.13	0.49
1:B:256:PRO:O	1:B:260:ILE:HG13	2.13	0.48
1:B:497:LEU:O	1:B:501:ILE:HG13	2.13	0.48
1:D:492:LEU:O	1:D:496:VAL:HG23	2.13	0.48
1:D:441:HIS:C	1:D:441:HIS:ND1	2.66	0.48
1:A:247:PRO:HD2	1:A:277:LEU:HB3	1.95	0.48
1:A:125:SER:OG	1:A:356:GLY:HA3	2.14	0.48
1:A:441:HIS:ND1	1:A:441:HIS:C	2.66	0.48
1:A:282:LEU:HB3	1:A:295:PHE:CE2	2.49	0.48
1:B:249:TYR:N	1:B:250:PRO:CD	2.76	0.48
1:B:282:LEU:HB3	1:B:295:PHE:CE2	2.48	0.48
1:C:249:TYR:N	1:C:250:PRO:CD	2.76	0.48
1:D:395:ILE:HD11	1:D:462:GLN:HG3	1.94	0.48
1:D:249:TYR:N	1:D:250:PRO:CD	2.76	0.48
1:D:63:ARG:HG3	1:D:63:ARG:O	2.14	0.48
1:C:170:GLU:OE2	1:C:349:THR:HB	2.13	0.48
1:D:247:PRO:HD2	1:D:277:LEU:HB3	1.96	0.48
1:C:192:PRO:HB3	1:C:240:VAL:HG11	1.95	0.47
1:D:154:ASP:C	1:D:156:ALA:H	2.17	0.47
1:A:395:ILE:HD11	1:A:462:GLN:HG3	1.96	0.47
1:C:117:GLU:HG2	1:D:81:LEU:HD13	1.95	0.47
1:C:125:SER:OG	1:C:356:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:GLU:OE2	1:D:349:THR:HB	2.14	0.47
2:A:514:PLR:H4A1	2:A:514:PLR:P	2.54	0.47
1:D:277:LEU:HA	1:D:277:LEU:HD12	1.73	0.47
1:B:192:PRO:HB3	1:B:240:VAL:HG11	1.97	0.47
1:D:284:TRP:HB3	1:D:375:LEU:HD13	1.96	0.47
1:A:192:PRO:HB3	1:A:240:VAL:HG11	1.97	0.47
1:A:81:LEU:HD13	1:B:117:GLU:HG2	1.97	0.47
1:B:154:ASP:C	1:B:156:ALA:H	2.17	0.47
1:A:92:SER:N	1:A:93:PRO:CD	2.77	0.46
1:D:385:ALA:O	1:D:389:LYS:HG3	2.14	0.46
1:B:284:TRP:CH2	1:B:371:GLU:HG2	2.51	0.46
1:B:63:ARG:HG3	1:B:63:ARG:O	2.15	0.46
1:C:336:ILE:HD13	1:D:497:LEU:HB3	1.97	0.46
1:C:284:TRP:CH2	1:C:371:GLU:HG2	2.50	0.46
1:C:385:ALA:O	1:C:389:LYS:HG3	2.15	0.46
1:C:81:LEU:HD13	1:D:117:GLU:HG2	1.98	0.46
1:A:284:TRP:CH2	1:A:371:GLU:HG2	2.51	0.46
1:C:63:ARG:HG3	1:C:63:ARG:O	2.15	0.46
1:C:492:LEU:O	1:C:496:VAL:HG23	2.15	0.45
1:C:69:ARG:HG2	1:D:149:HIS:CD2	2.51	0.45
1:D:192:PRO:HB3	1:D:240:VAL:HG11	1.98	0.45
1:A:310:HIS:HB2	1:A:317:LYS:HA	1.99	0.45
1:A:395:ILE:HA	1:A:396:PRO:HD3	1.72	0.45
1:A:69:ARG:HG2	1:B:149:HIS:CD2	2.50	0.45
1:D:284:TRP:HH2	1:D:371:GLU:HG2	1.81	0.45
1:A:135:SER:HB3	1:B:91:GLU:OE2	2.16	0.45
1:D:292:VAL:O	1:D:292:VAL:CG2	2.65	0.45
1:B:292:VAL:O	1:B:292:VAL:CG2	2.64	0.45
1:B:395:ILE:HD11	1:B:462:GLN:HG3	1.99	0.45
1:C:292:VAL:O	1:C:292:VAL:CG2	2.64	0.45
1:D:310:HIS:HB2	1:D:317:LYS:HA	1.99	0.45
1:D:92:SER:N	1:D:93:PRO:CD	2.80	0.45
1:B:247:PRO:HD2	1:B:277:LEU:HB3	1.98	0.45
1:C:284:TRP:HB3	1:C:375:LEU:HD13	1.99	0.45
1:A:284:TRP:HB3	1:A:375:LEU:HD13	1.98	0.45
1:A:63:ARG:O	1:A:63:ARG:HG3	2.17	0.45
1:C:247:PRO:HD2	1:C:277:LEU:HB3	1.99	0.44
1:C:395:ILE:HD11	1:C:462:GLN:HG3	1.98	0.44
1:D:497:LEU:O	1:D:501:ILE:HG13	2.16	0.44
1:B:385:ALA:O	1:B:389:LYS:HG3	2.16	0.44
1:A:385:ALA:O	1:A:389:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:SER:N	1:C:93:PRO:CD	2.81	0.44
1:B:92:SER:N	1:B:93:PRO:CD	2.80	0.44
1:B:196:VAL:HG12	1:B:243:ALA:HB3	2.00	0.43
1:C:431:LEU:HD13	1:C:440:PHE:CE1	2.53	0.43
1:A:431:LEU:HD13	1:A:440:PHE:CE1	2.54	0.43
1:C:310:HIS:HB2	1:C:317:LYS:HA	2.00	0.43
1:D:127:PRO:HD2	1:D:354:ARG:HB2	2.00	0.43
1:D:395:ILE:HA	1:D:396:PRO:HD3	1.72	0.43
1:D:252:GLY:HA3	1:D:407:VAL:HB	2.00	0.43
1:C:431:LEU:HD13	1:C:440:PHE:CD1	2.53	0.43
1:C:429:TRP:CH2	1:C:457:PHE:HB2	2.54	0.43
1:C:127:PRO:HD2	1:C:354:ARG:HB2	2.00	0.43
1:A:149:HIS:CD2	1:B:69:ARG:HG2	2.54	0.43
1:A:492:LEU:O	1:A:496:VAL:HG23	2.18	0.43
1:A:57:ILE:O	1:A:59:PRO:HD3	2.19	0.43
1:A:292:VAL:CG2	1:A:292:VAL:O	2.66	0.43
1:C:497:LEU:HA	1:C:497:LEU:HD12	1.89	0.43
1:C:335:PHE:CD2	1:D:206:LYS:HE2	2.54	0.43
1:B:288:LEU:HD13	1:B:375:LEU:HD11	2.01	0.42
1:D:419:GLN:O	1:D:423:GLU:HG2	2.19	0.42
1:D:429:TRP:CH2	1:D:457:PHE:HB2	2.54	0.42
1:A:419:GLN:O	1:A:423:GLU:HG2	2.18	0.42
1:B:431:LEU:HD13	1:B:440:PHE:CD1	2.55	0.42
1:A:252:GLY:HA3	1:A:407:VAL:HB	2.01	0.42
1:B:310:HIS:HB2	1:B:317:LYS:HA	2.00	0.42
1:B:492:LEU:O	1:B:496:VAL:HG23	2.18	0.42
4:B:514:EXT:HAV	5:B:516:HOH:O	2.19	0.42
1:D:497:LEU:HA	1:D:497:LEU:HD12	1.89	0.42
1:A:91:GLU:OE2	1:B:135:SER:HB3	2.19	0.42
1:C:196:VAL:HG12	1:C:243:ALA:HB3	2.00	0.42
1:C:284:TRP:HH2	1:C:371:GLU:HG2	1.84	0.42
1:C:419:GLN:O	1:C:423:GLU:HG2	2.19	0.42
1:D:57:ILE:O	1:D:59:PRO:HD3	2.20	0.42
1:B:58:LYS:HA	1:B:59:PRO:HD3	1.88	0.42
1:C:277:LEU:HA	1:C:277:LEU:HD12	1.75	0.41
1:C:371:GLU:O	1:C:375:LEU:HB2	2.20	0.41
1:C:206:LYS:HE2	1:D:335:PHE:CD2	2.55	0.41
1:A:429:TRP:CH2	1:A:457:PHE:HB2	2.55	0.41
1:B:419:GLN:O	1:B:423:GLU:HG2	2.20	0.41
1:C:57:ILE:O	1:C:59:PRO:HD3	2.20	0.41
1:B:284:TRP:HB3	1:B:375:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:HD13	1:B:440:PHE:CE1	2.55	0.41
1:C:252:GLY:HA3	1:C:407:VAL:HB	2.02	0.41
1:A:284:TRP:HH2	1:A:371:GLU:HG2	1.84	0.41
1:A:431:LEU:HD13	1:A:440:PHE:CD1	2.54	0.41
1:B:429:TRP:CH2	1:B:457:PHE:HB2	2.56	0.41
1:D:431:LEU:HD13	1:D:440:PHE:CE1	2.56	0.41
1:B:284:TRP:HH2	1:B:371:GLU:HG2	1.85	0.41
1:B:252:GLY:HA3	1:B:407:VAL:HB	2.03	0.41
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.76	0.41
1:C:174:LEU:HD22	1:C:333:GLN:HG3	2.03	0.41
1:C:106:HIS:CE1	1:C:108:ASP:HB3	2.56	0.40
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.87	0.40
1:C:329:LEU:HD12	1:C:329:LEU:HA	1.87	0.40
1:B:170:GLU:HB2	5:B:523:HOH:O	2.21	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	451/514 (88%)	430 (95%)	19 (4%)	2 (0%)	34	66
1	B	451/514 (88%)	430 (95%)	19 (4%)	2 (0%)	34	66
1	C	450/514 (88%)	428 (95%)	20 (4%)	2 (0%)	34	66
1	D	450/514 (88%)	430 (96%)	18 (4%)	2 (0%)	34	66
All	All	1802/2056 (88%)	1718 (95%)	76 (4%)	8 (0%)	34	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA

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Mol	Chain	Res	Type
1	C	155	ALA
1	B	155	ALA
1	D	103	ALA
1	A	103	ALA
1	B	103	ALA
1	C	103	ALA
1	D	155	ALA

### 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	339/395 (86%)	321 (95%)	18 (5%)	22	54
1	B	339/395 (86%)	320 (94%)	19 (6%)	21	52
1	C	338/395 (86%)	321 (95%)	17 (5%)	24	57
1	D	338/395 (86%)	318 (94%)	20 (6%)	19	49
All	All	1354/1580 (86%)	1280 (94%)	74 (6%)	21	53

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	128	LEU
1	A	263	LEU
1	A	282	LEU
1	A	292	VAL
1	A	310	HIS
1	A	330	LEU
1	A	375	LEU
1	A	405	LEU
1	A	410	VAL
1	A	436	ARG
1	A	441	HIS
1	A	446	LEU
1	A	461	LEU

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Mol	Chain	Res	Type
1	A	492	LEU
1	A	494	ARG
1	A	497	LEU
1	A	503	LEU
1	B	128	LEU
1	B	154	ASP
1	B	263	LEU
1	B	282	LEU
1	B	288	LEU
1	B	292	VAL
1	B	310	HIS
1	B	330	LEU
1	B	375	LEU
1	B	405	LEU
1	B	410	VAL
1	B	436	ARG
1	B	441	HIS
1	B	446	LEU
1	B	461	LEU
1	B	492	LEU
1	B	494	ARG
1	B	497	LEU
1	B	503	LEU
1	C	128	LEU
1	C	263	LEU
1	C	282	LEU
1	C	292	VAL
1	C	310	HIS
1	C	330	LEU
1	C	375	LEU
1	C	405	LEU
1	C	410	VAL
1	C	436	ARG
1	C	441	HIS
1	C	446	LEU
1	C	461	LEU
1	C	492	LEU
1	C	494	ARG
1	C	497	LEU
1	C	503	LEU
1	D	128	LEU
1	D	154	ASP

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Mol	Chain	Res	Type
1	D	263	LEU
1	D	282	LEU
1	D	288	LEU
1	D	292	VAL
1	D	310	HIS
1	D	330	LEU
1	D	375	LEU
1	D	383	GLN
1	D	405	LEU
1	D	410	VAL
1	D	436	ARG
1	D	441	HIS
1	D	446	LEU
1	D	461	LEU
1	D	492	LEU
1	D	494	ARG
1	D	497	LEU
1	D	503	LEU

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

Mol	Chain	Res	Type
1	C	435	HIS
1	D	435	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

5 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$
4	EXT	D	514	-	23,23,23	1.70	4 (17%)	30,33,33	1.18	2 (6%)
3	PO4	A	515	-	4,4,4	0.88	0	6,6,6	0.42	0
2	PLR	A	514	-	15,15,15	1.02	1 (6%)	20,22,22	1.12	1 (5%)
4	EXT	B	514	-	23,23,23	1.67	4 (17%)	30,33,33	1.27	3 (10%)
4	EXT	C	514	-	23,23,23	1.73	5 (21%)	30,33,33	1.46	4 (13%)

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
4	EXT	D	514	-	-	9/15/15/15	0/1/1/1
4	EXT	C	514	-	-	8/15/15/15	0/1/1/1
2	PLR	A	514	-	-	0/6/6/6	0/1/1/1
4	EXT	B	514	-	-	7/15/15/15	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	514	EXT	PAQ-OAS	4.74	1.65	1.50
4	C	514	EXT	PAQ-OAS	4.51	1.65	1.50
4	D	514	EXT	PAQ-OAS	4.24	1.64	1.50
4	D	514	EXT	CAA-CAB	-3.80	1.39	1.46
4	C	514	EXT	CAA-CAB	-3.76	1.39	1.46
4	B	514	EXT	CAA-CAB	-3.49	1.40	1.46
4	D	514	EXT	PAQ-OAP	2.79	1.65	1.54
4	C	514	EXT	PAC-OAD	2.60	1.64	1.54
2	A	514	PLR	C2-N1	2.54	1.38	1.33
4	C	514	EXT	PAQ-OAP	2.49	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	514	EXT	PAQ-OAP	2.26	1.63	1.54
4	B	514	EXT	PAC-OAD	2.11	1.63	1.54
4	C	514	EXT	PAC-OAF	2.10	1.62	1.54
4	D	514	EXT	CAA-CAI	-2.00	1.39	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	514	EXT	CAU-CAV-NAW	-3.65	105.18	111.12
4	B	514	EXT	OAR-PAQ-OAT	3.15	115.12	106.73
4	D	514	EXT	OAG-PAC-OAE	3.05	115.03	106.47
4	D	514	EXT	OAR-PAQ-OAT	2.96	114.61	106.73
4	C	514	EXT	OAR-PAQ-OAT	2.63	113.74	106.73
2	A	514	PLR	C6-C5-C4	2.59	120.20	118.16
4	B	514	EXT	OAG-PAC-OAE	2.53	113.56	106.47
4	C	514	EXT	OAG-CAH-CAI	2.39	113.91	109.35
4	B	514	EXT	CAH-CAI-CAK	-2.31	115.57	119.37
4	C	514	EXT	OAG-PAC-OAE	2.15	112.50	106.47

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	514	EXT	CAH-OAG-PAC-OAD
4	D	514	EXT	CAU-OAT-PAQ-OAP
4	D	514	EXT	CAU-OAT-PAQ-OAR
4	D	514	EXT	CAU-OAT-PAQ-OAS
4	D	514	EXT	OAT-CAU-CAV-NAW
4	D	514	EXT	CAU-CAV-NAW-CAB
4	B	514	EXT	CAI-CAA-CAB-NAW
4	B	514	EXT	CAU-OAT-PAQ-OAP
4	B	514	EXT	CAU-OAT-PAQ-OAR
4	B	514	EXT	CAU-OAT-PAQ-OAS
4	B	514	EXT	CAU-CAV-NAW-CAB
4	C	514	EXT	CAH-OAG-PAC-OAD
4	C	514	EXT	CAH-OAG-PAC-OAF
4	C	514	EXT	OAT-CAU-CAV-NAW
4	C	514	EXT	CAU-CAV-NAW-CAB
4	C	514	EXT	CAN-CAA-CAB-NAW
4	B	514	EXT	CAN-CAA-CAB-NAW
4	C	514	EXT	CAH-OAG-PAC-OAE
4	D	514	EXT	CAN-CAA-CAB-NAW

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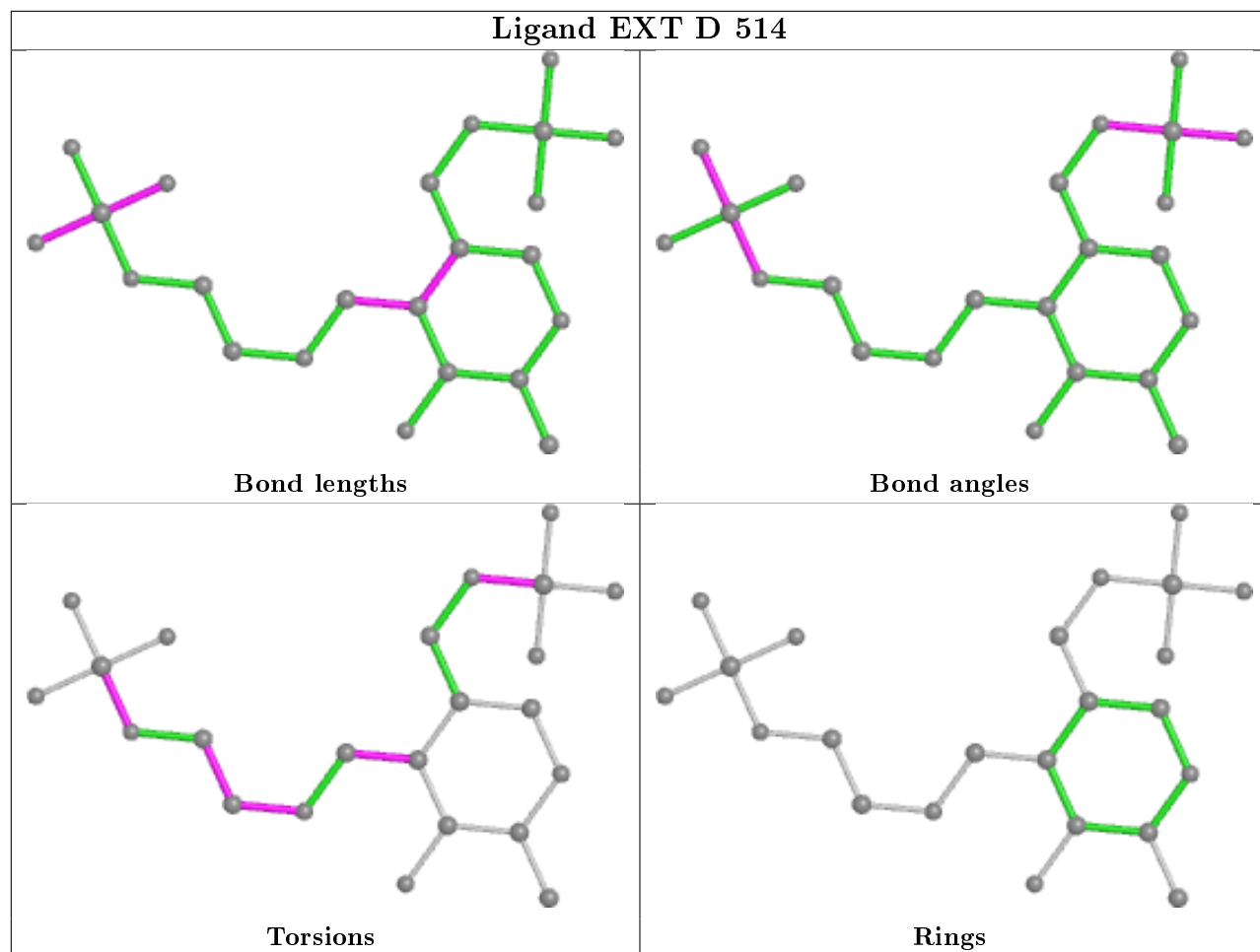
Mol	Chain	Res	Type	Atoms
4	D	514	EXT	CAI-CAA-CAB-NAW
4	B	514	EXT	CAV-CAU-OAT-PAQ
4	C	514	EXT	CAU-OAT-PAQ-OAS
4	D	514	EXT	CAH-OAG-PAC-OAF
4	C	514	EXT	CAI-CAA-CAB-NAW

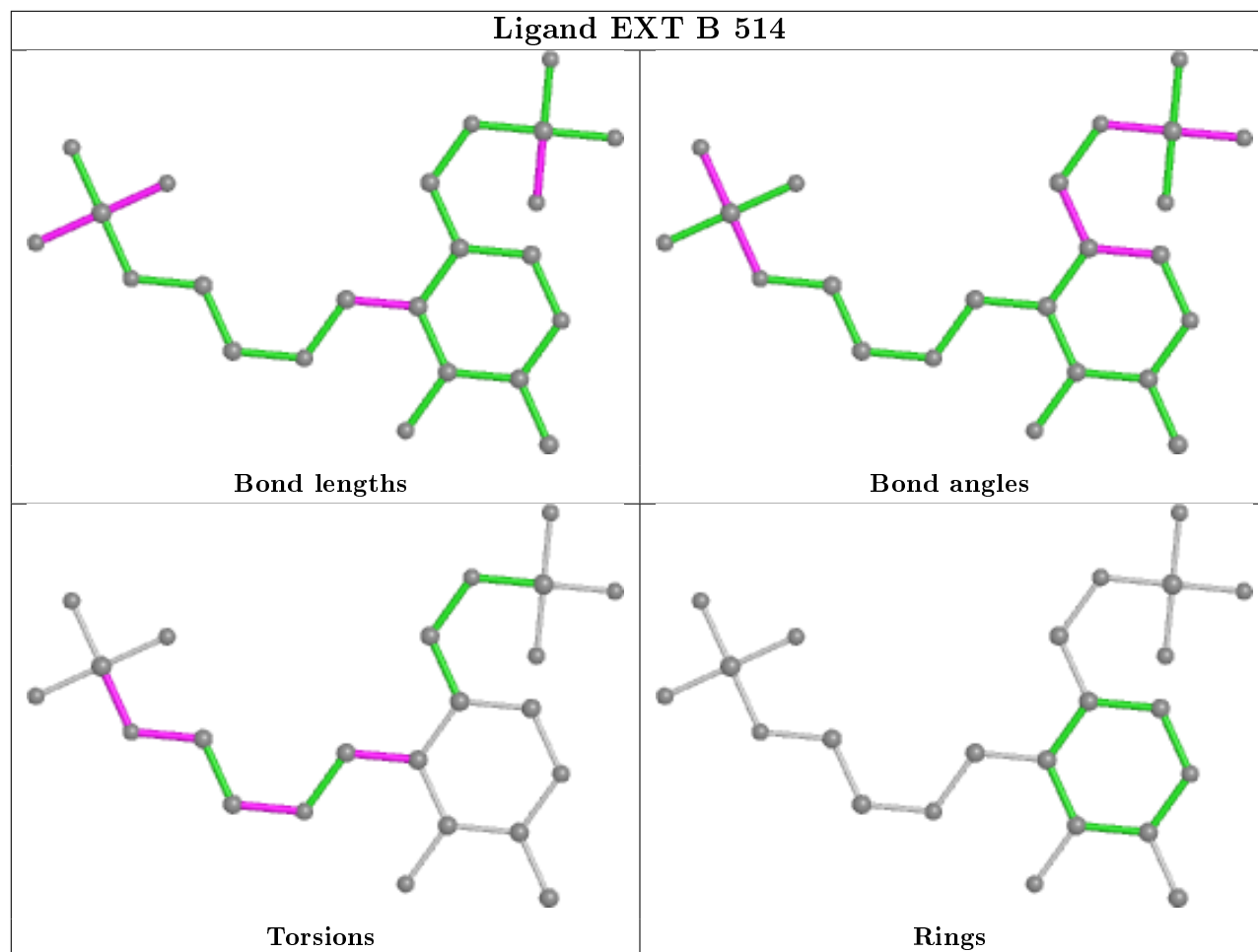
There are no ring outliers.

2 monomers are involved in 3 short contacts:

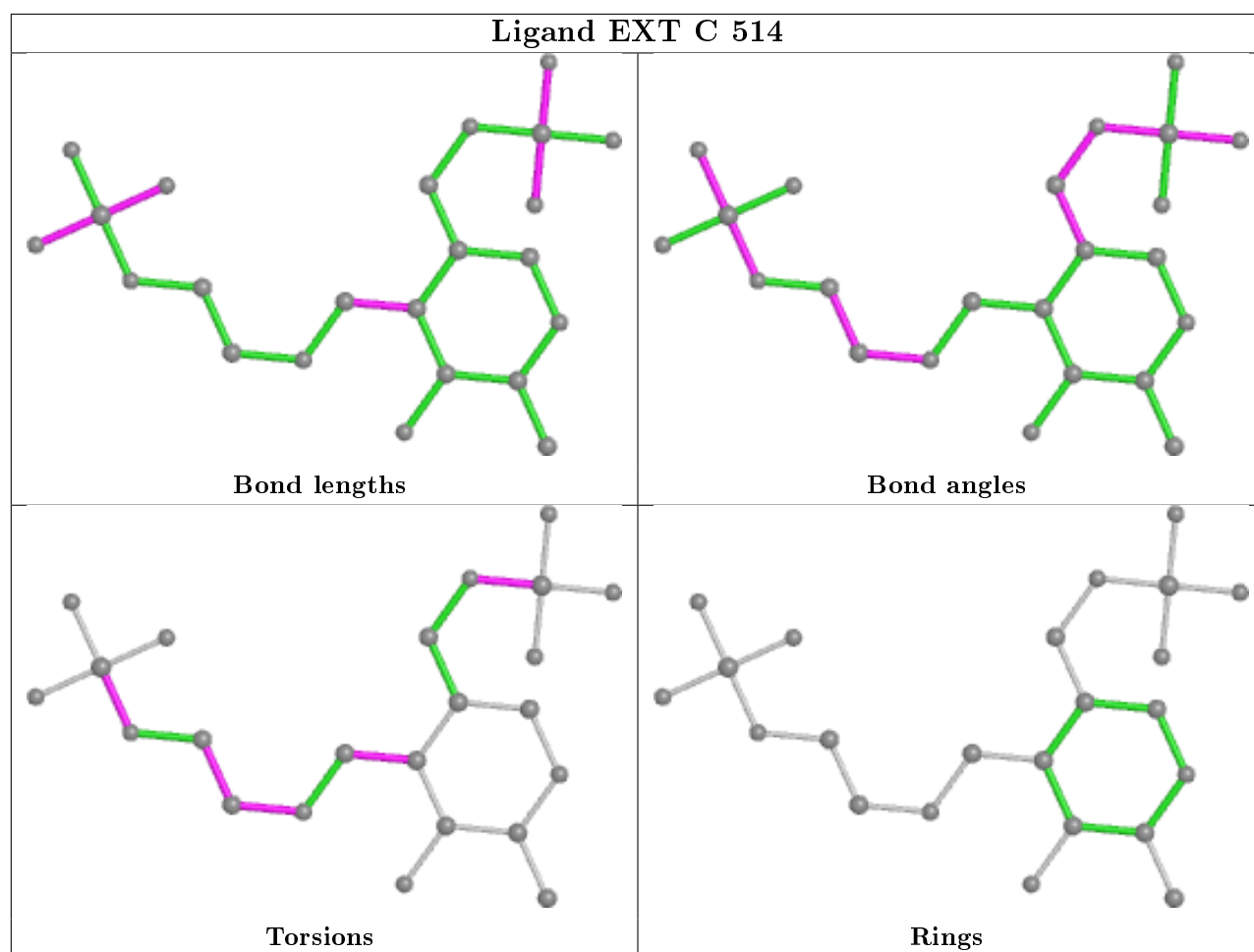
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	514	PLR	2	0
4	B	514	EXT	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	452/514 (87%)	-0.04	1 (0%) 95 95	54, 70, 86, 104	0
1	B	451/514 (87%)	-0.11	4 (0%) 84 84	54, 70, 86, 101	0
1	C	452/514 (87%)	-0.09	6 (1%) 77 77	55, 70, 86, 111	0
1	D	452/514 (87%)	0.01	10 (2%) 62 59	54, 70, 86, 101	0
All	All	1807/2056 (87%)	-0.06	21 (1%) 79 79	54, 70, 86, 111	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	SER	3.7
1	C	508	HIS	3.6
1	D	289	GLY	3.4
1	D	214	LYS	2.8
1	C	61	ARG	2.8
1	D	60	TYR	2.8
1	C	506	GLU	2.8
1	D	61	ARG	2.7
1	C	473	GLU	2.6
1	D	473	GLU	2.6
1	B	274	ASP	2.6
1	A	61	ARG	2.4
1	D	306	SER	2.4
1	C	306	SER	2.2
1	D	286	GLU	2.2
1	B	304	SER	2.2
1	D	399	LYS	2.1
1	D	411	ALA	2.1
1	C	500	PHE	2.1
1	D	276	CYS	2.1
1	B	276	CYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

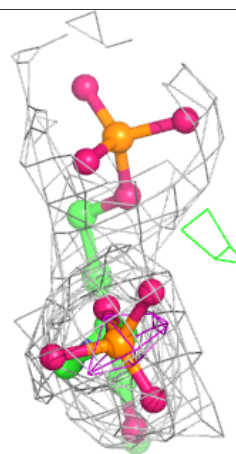
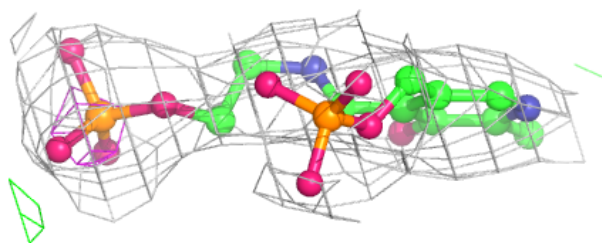
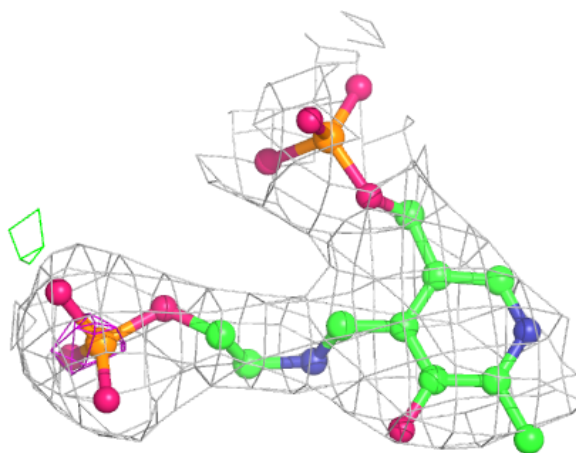
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	PO4	A	515	5/5	0.94	0.17	70,73,80,81	0
4	EXT	D	514	23/23	0.95	0.17	53,63,72,82	0
4	EXT	B	514	23/23	0.95	0.17	54,60,76,82	0
4	EXT	C	514	23/23	0.95	0.16	60,64,78,87	0
2	PLR	A	514	15/15	0.97	0.15	56,58,61,62	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.

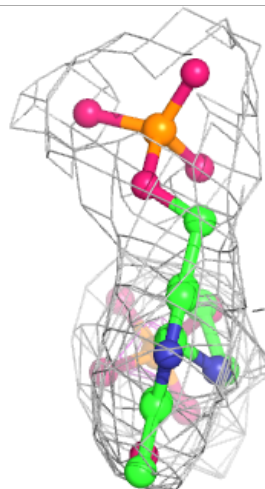
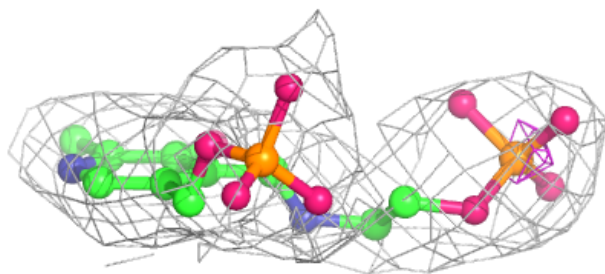
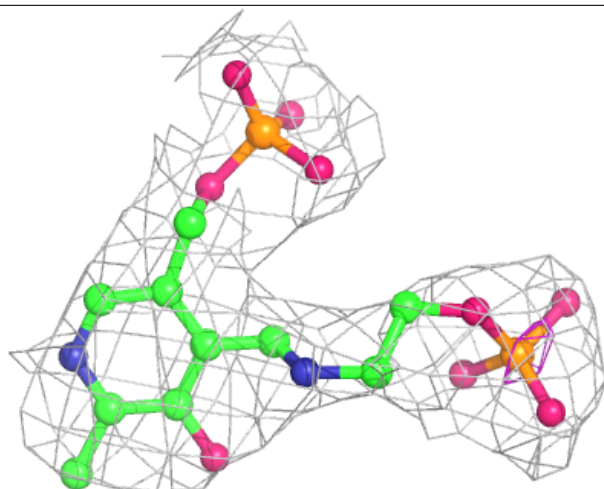
**Electron density around EXT D 514:**

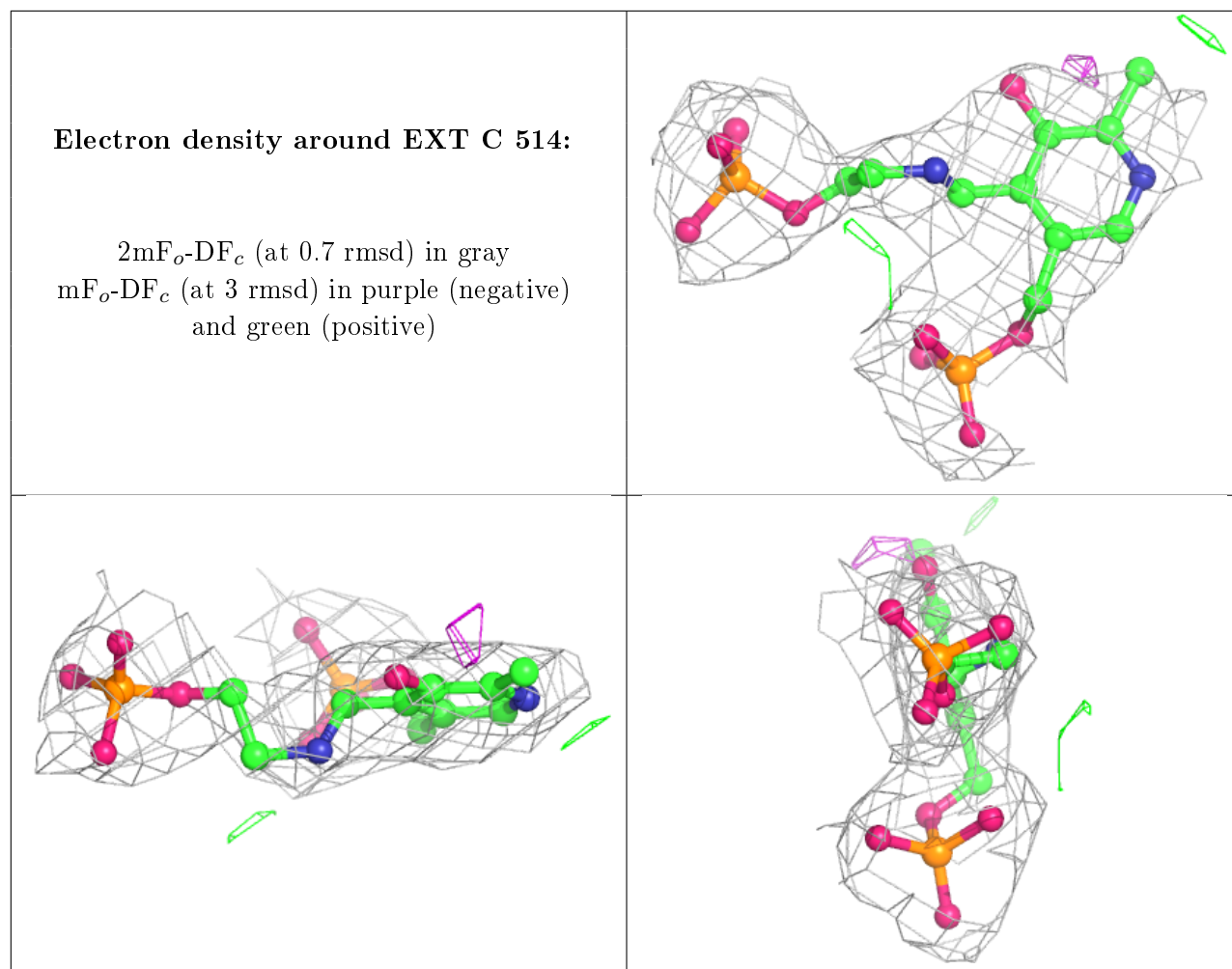
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around EXT B 514:**

$2mF_o-DF_c$  (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.