



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:05 AM BST

PDB ID : 5L6S  
Title : Crystal structure of E. coli ADP-glucose pyrophosphorylase (AGPase) in complex with a positive allosteric regulator beta-fructose-1,6-diphosphate (FBP) - AGPase\*FBP  
Authors : Cifuentes, J.O.; Albasa-Jove, D.; Comino, N.; Madariaga-Marcos, J.; Agirre, J.; Lopez-Fernandez, S.; Garcia-Alija, M.; Guerin, M.E.  
Deposited on : 2016-05-31  
Resolution : 3.04 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

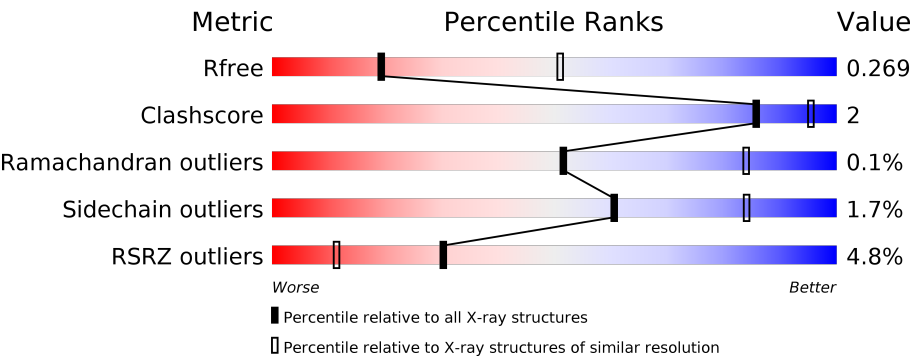
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 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	431	<div><div>3%</div><div><div></div><div>90%</div><div></div><div>5%</div></div></div>
1	B	431	<div><div></div><div><div></div><div>89%</div><div></div><div>7%</div><div></div></div></div>
1	C	431	<div><div></div><div><div></div><div>88%</div><div></div><div>8%</div><div></div></div></div>
1	D	431	<div><div>3%</div><div><div></div><div>87%</div><div></div><div>6%</div><div>7%</div></div></div>
1	E	431	<div><div>%</div><div><div></div><div>88%</div><div></div><div>7%</div><div>5%</div></div></div>
1	F	431	<div><div>2%</div><div><div></div><div>87%</div><div></div><div>6%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	431	
1	H	431	
1	I	431	
1	J	431	
1	K	431	
1	L	431	
1	M	431	
1	N	431	
1	O	431	
1	P	431	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	E	501	-	-	X	-
2	SO4	F	501	-	-	X	-
2	SO4	I	501	-	-	X	-
2	SO4	J	501	-	-	X	-
2	SO4	K	503	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45056 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 Glucose-1-phosphate adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3016	1913	518	567	18			
1	B	417	Total	C	N	O	S	0	0	0
			3194	2023	563	588	20			
1	C	418	Total	C	N	O	S	0	0	0
			3283	2071	580	611	21			
1	D	402	Total	C	N	O	S	0	0	0
			2938	1849	521	550	18			
1	E	408	Total	C	N	O	S	0	0	0
			3108	1969	544	575	20			
1	F	402	Total	C	N	O	S	0	0	0
			3059	1929	541	570	19			
1	G	409	Total	C	N	O	S	0	0	0
			3144	1988	551	585	20			
1	H	408	Total	C	N	O	S	0	0	0
			3076	1955	536	565	20			
1	I	409	Total	C	N	O	S	0	0	0
			3138	1983	551	585	19			
1	J	407	Total	C	N	O	S	0	0	0
			3074	1942	536	577	19			
1	K	409	Total	C	N	O	S	0	0	0
			3115	1966	546	583	20			
1	L	415	Total	C	N	O	S	0	0	0
			3196	2020	558	598	20			
1	M	229	Total	C	N	O		0	0	0
			1185	703	242	240				
1	N	369	Total	C	N	O	S	0	0	0
			2278	1416	407	443	12			
1	O	364	Total	C	N	O	S	0	0	0
			2145	1348	385	407	5			
1	P	339	Total	C	N	O	S	0	0	0
			1832	1096	367	361	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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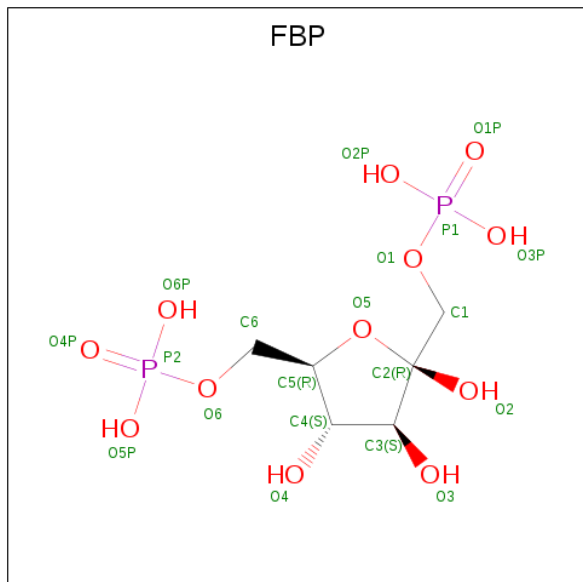
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).

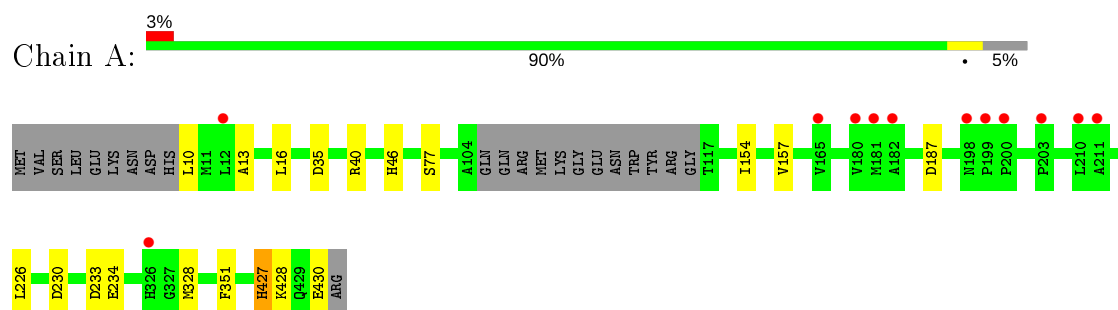


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	P	0	0
			20	6	12	2		
3	G	1	Total	C	O	P	0	0
			20	6	12	2		
3	I	1	Total	C	O	P	0	0
			20	6	12	2		
3	L	1	Total	C	O	P	0	0
			20	6	12	2		

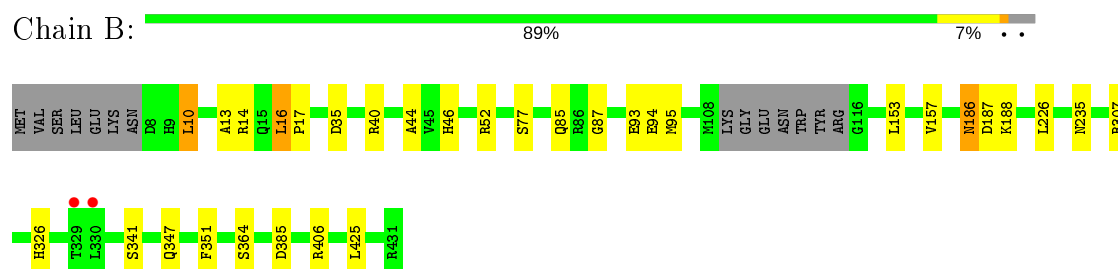
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

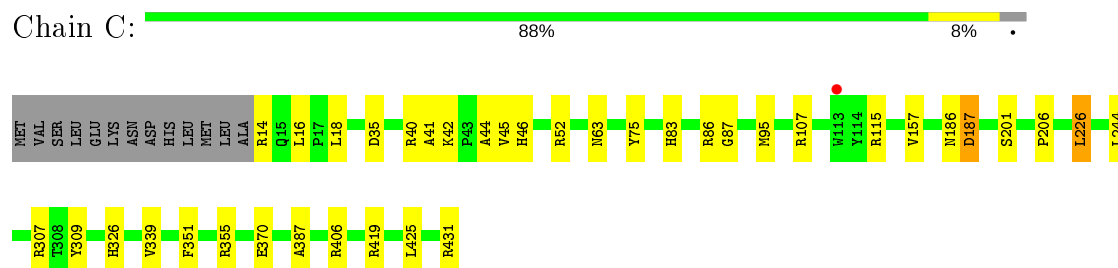
- Molecule 1: Glucose-1-phosphate adenylyltransferase



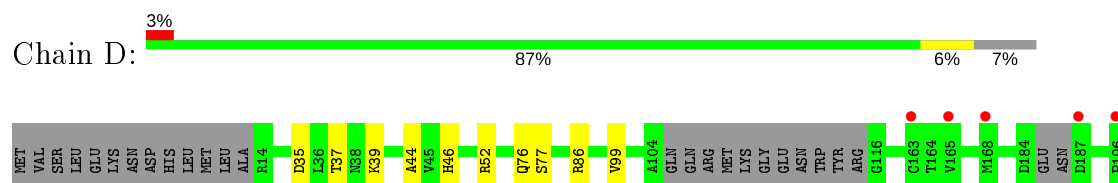
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase



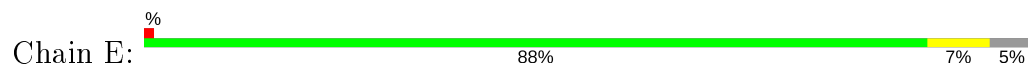
- Molecule 1: Glucose-1-phosphate adenylyltransferase



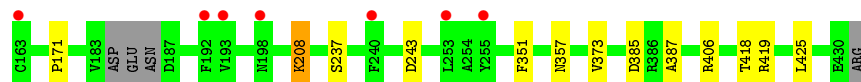
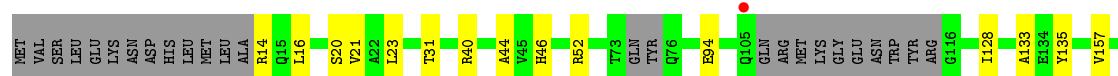
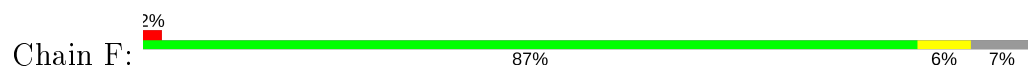




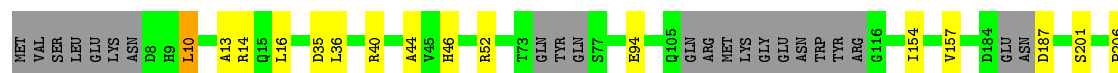
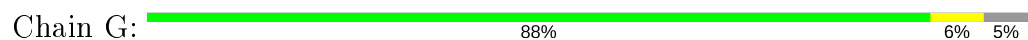
- Molecule 1: Glucose-1-phosphate adenylyltransferase



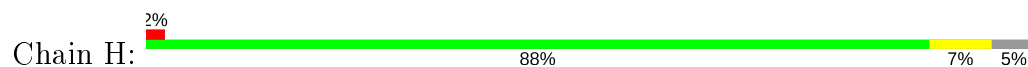
- Molecule 1: Glucose-1-phosphate adenylyltransferase



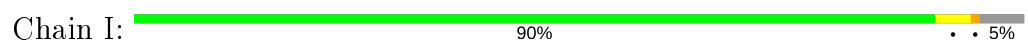
- Molecule 1: Glucose-1-phosphate adenylyltransferase

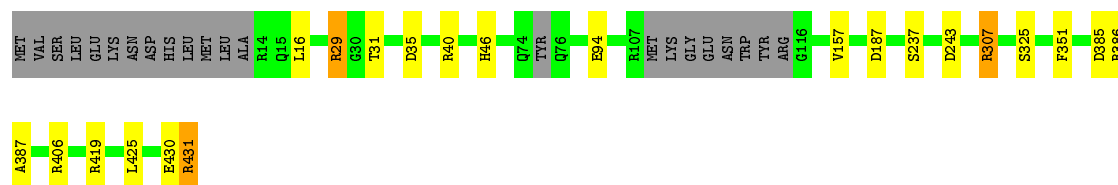


- Molecule 1: Glucose-1-phosphate adenylyltransferase

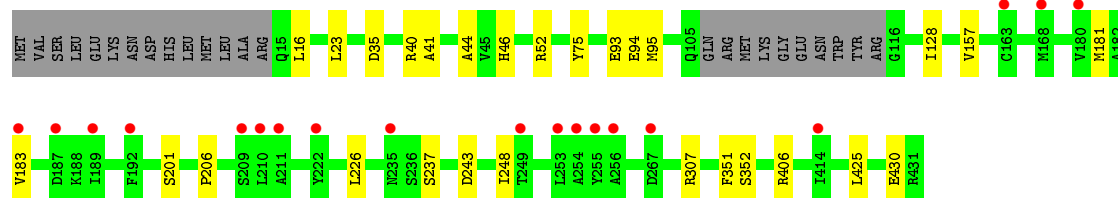
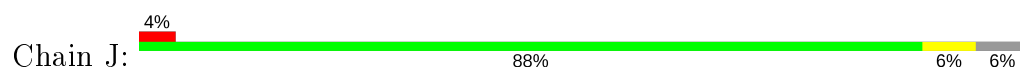


- Molecule 1: Glucose-1-phosphate adenylyltransferase

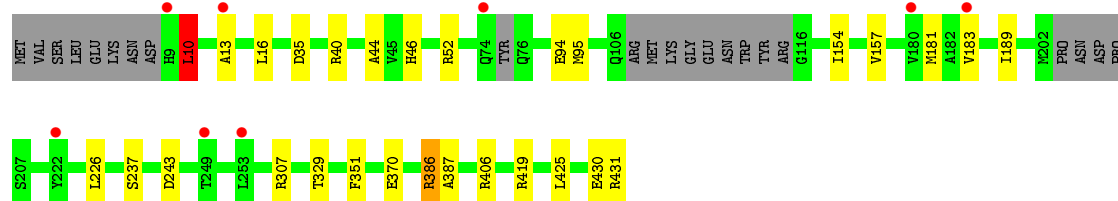
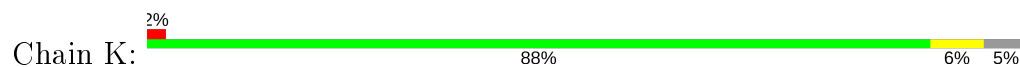




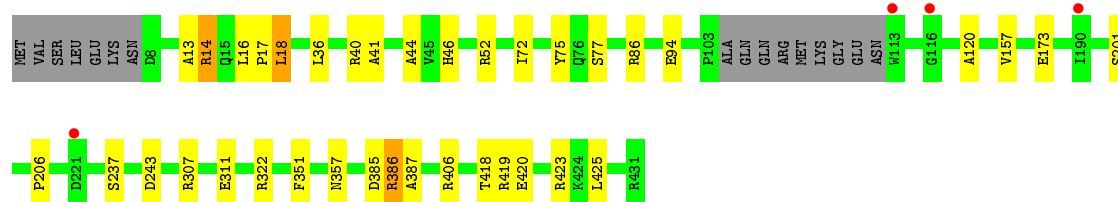
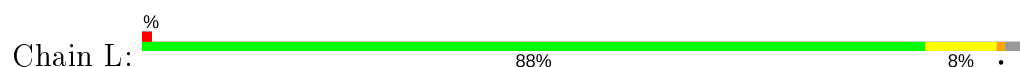
- Molecule 1: Glucose-1-phosphate adenylyltransferase



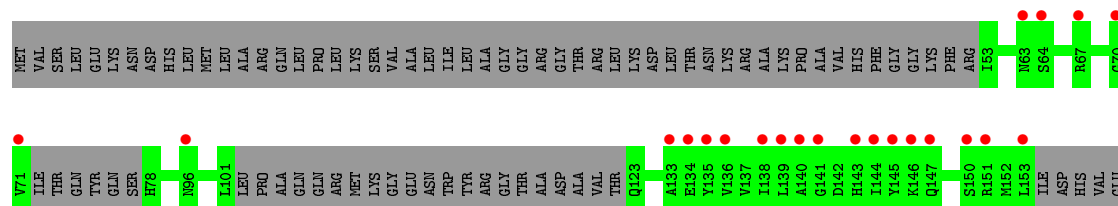
- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase



- Molecule 1: Glucose-1-phosphate adenylyltransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.16Å 148.90Å 177.49Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	70.75 – 3.04 70.75 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.7 (70.75-3.04) 98.6 (70.75-3.04)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX (dev_2219: ???)	Depositor
R, $R_{free}$	0.234 , 0.272 0.231 , 0.269	Depositor DCC
$R_{free}$ test set	7259 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.0	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	0.92	EDS
Total number of atoms	45056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, SO4

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	0.24	0/3083	0.42	0/4212
1	B	0.24	0/3261	0.42	0/4428
1	C	0.25	0/3354	0.42	0/4546
1	D	0.25	0/2997	0.43	0/4083
1	E	0.25	0/3174	0.42	0/4311
1	F	0.24	0/3121	0.42	0/4240
1	G	0.25	0/3208	0.43	1/4353 (0.0%)
1	H	0.24	0/3142	0.42	0/4276
1	I	0.25	0/3203	0.43	0/4349
1	J	0.24	0/3140	0.42	0/4277
1	K	0.25	0/3176	0.44	1/4314 (0.0%)
1	L	0.25	0/3263	0.42	0/4431
1	M	0.23	0/1186	0.43	0/1642
1	N	0.24	0/2312	0.43	0/3186
1	O	0.25	0/2186	0.42	0/3030
1	P	0.24	0/1841	0.43	0/2542
All	All	0.24	0/45647	0.43	2/62220 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	10	LEU	CA-CB-CG	7.33	132.16	115.30
1	G	10	LEU	CA-CB-CG	5.11	127.05	115.30

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	3016	0	2779	9	0
1	B	3194	0	3112	20	0
1	C	3283	0	3215	23	0
1	D	2938	0	2718	16	0
1	E	3108	0	2996	17	1
1	F	3059	0	2944	18	0
1	G	3144	0	3050	17	0
1	H	3076	0	2942	13	0
1	I	3138	0	3038	12	1
1	J	3074	0	2918	15	0
1	K	3115	0	2991	15	0
1	L	3196	0	3093	21	0
1	M	1185	0	606	1	0
1	N	2278	0	1714	4	0
1	O	2145	0	1418	0	0
1	P	1832	0	1096	3	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	1	0
2	D	20	0	0	1	0
2	E	15	0	0	3	0
2	F	10	0	0	3	0
2	G	15	0	0	1	0
2	H	20	0	0	0	0
2	I	15	0	0	2	0
2	J	15	0	0	2	0
2	K	15	0	0	2	0
2	L	15	0	0	2	0
2	P	10	0	0	0	0
3	C	20	0	10	0	0
3	G	20	0	10	1	0
3	I	20	0	10	0	0
3	L	20	0	10	1	0
All	All	45056	0	40670	186	1

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 2.

All (186) 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:87:GLY:O	1:B:307:ARG:NH1	2.18	0.75
1:B:186:ASN:O	1:B:188:LYS:N	2.20	0.74
1:C:87:GLY:O	1:C:307:ARG:NH2	2.21	0.74
1:B:307:ARG:HB3	1:C:95:MET:HE3	1.70	0.73
1:G:36:LEU:O	1:G:40:ARG:NH1	2.21	0.73
1:E:40:ARG:NH1	2:E:501:SO4:S	2.64	0.71
1:B:16:LEU:HD12	1:B:153:LEU:HB3	1.74	0.69
1:B:40:ARG:NH2	1:B:385:ASP:OD1	2.26	0.69
1:G:13:ALA:HB2	1:G:154:ILE:HD11	1.73	0.69
1:E:40:ARG:NH1	2:E:501:SO4:O3	2.26	0.69
1:F:40:ARG:NH1	2:F:501:SO4:O4	2.26	0.69
1:L:36:LEU:O	1:L:40:ARG:NH1	2.27	0.66
1:F:40:ARG:NH1	2:F:501:SO4:S	2.69	0.66
1:D:370:GLU:O	1:D:431:ARG:NH2	2.28	0.66
1:J:95:MET:HE3	1:K:307:ARG:HB3	1.78	0.64
1:I:46:HIS:NE2	2:I:501:SO4:O4	2.30	0.63
1:B:40:ARG:NH1	2:B:503:SO4:O1	2.31	0.63
1:I:29:ARG:HG3	1:I:31:THR:HG23	1.81	0.62
1:E:13:ALA:O	1:E:17:PRO:HD2	2.00	0.62
1:E:40:ARG:NH1	2:E:501:SO4:O4	2.32	0.61
1:J:40:ARG:NH1	2:J:501:SO4:S	2.74	0.60
1:J:40:ARG:NH1	2:J:501:SO4:O3	2.35	0.60
1:G:40:ARG:NH2	1:G:385:ASP:OD1	2.34	0.60
1:L:13:ALA:O	1:L:17:PRO:HD2	2.03	0.59
1:F:14:ARG:HG3	1:G:14:ARG:HG3	1.86	0.58
1:C:406:ARG:HB3	1:C:425:LEU:HD21	1.86	0.58
1:L:44:ALA:O	1:L:52:ARG:NH1	2.35	0.58
1:F:21:VAL:HG23	1:F:133:ALA:HB2	1.85	0.57
1:I:16:LEU:HD21	1:I:157:VAL:HG21	1.86	0.57
1:E:17:PRO:HB3	1:E:66:ILE:HG12	1.86	0.57
1:G:16:LEU:HD21	1:G:157:VAL:HG21	1.87	0.57
1:J:16:LEU:HD21	1:J:157:VAL:HG21	1.87	0.57
1:B:85:GLN:NE2	1:D:99:VAL:O	2.39	0.56
1:H:387:ALA:O	1:H:419:ARG:NH1	2.38	0.56
1:E:420:GLU:OE2	1:E:423:ARG:NH2	2.39	0.55
1:H:406:ARG:HB3	1:H:425:LEU:HD21	1.89	0.55
1:I:387:ALA:O	1:I:419:ARG:NH1	2.38	0.55
1:E:189:ILE:HG13	1:E:254:ALA:HB3	1.89	0.55
1:H:13:ALA:HB2	1:H:154:ILE:HD11	1.89	0.55
1:F:406:ARG:HB3	1:F:425:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:ALA:O	1:C:419:ARG:NH1	2.37	0.55
1:G:406:ARG:HB3	1:G:425:LEU:HD21	1.89	0.54
1:K:406:ARG:HB3	1:K:425:LEU:HD21	1.89	0.54
1:I:406:ARG:HB3	1:I:425:LEU:HD11	1.89	0.54
1:D:44:ALA:O	1:D:52:ARG:NH1	2.41	0.54
1:J:237:SER:OG	1:J:243:ASP:OD2	2.22	0.54
1:A:16:LEU:HD21	1:A:157:VAL:HG21	1.90	0.54
1:A:13:ALA:HB2	1:A:154:ILE:HD11	1.90	0.53
1:F:16:LEU:HD21	1:F:157:VAL:HG21	1.89	0.53
1:G:386:ARG:NH2	2:G:501:SO4:O1	2.41	0.53
1:K:13:ALA:HB2	1:K:154:ILE:HD11	1.90	0.53
1:E:189:ILE:HB	1:E:249:THR:HG23	1.91	0.53
1:F:237:SER:OG	1:F:243:ASP:OD2	2.20	0.53
1:G:387:ALA:O	1:G:419:ARG:NH1	2.39	0.52
1:D:430:GLU:HA	1:D:431:ARG:CB	2.39	0.52
1:D:39:LYS:HA	1:D:76:GLN:HG2	1.91	0.52
1:B:406:ARG:HB3	1:B:425:LEU:HD21	1.92	0.52
1:D:430:GLU:HA	1:D:431:ARG:HB3	1.92	0.52
1:L:406:ARG:HB3	1:L:425:LEU:HD21	1.91	0.51
1:B:235:ASN:HD21	1:G:423:ARG:HD2	1.74	0.51
1:H:13:ALA:O	1:H:17:PRO:HD2	2.10	0.51
1:H:36:LEU:O	1:H:40:ARG:NH1	2.43	0.51
1:J:23:LEU:HD21	1:J:128:ILE:HD13	1.92	0.51
1:K:44:ALA:O	1:K:52:ARG:NH1	2.38	0.51
1:K:237:SER:OG	1:K:243:ASP:OD2	2.26	0.51
1:I:237:SER:OG	1:I:243:ASP:OD2	2.24	0.51
1:J:406:ARG:HB3	1:J:425:LEU:HD21	1.92	0.50
1:I:40:ARG:NH1	2:I:501:SO4:S	2.84	0.50
1:F:23:LEU:HD21	1:F:128:ILE:HD13	1.93	0.50
1:J:44:ALA:O	1:J:52:ARG:NH1	2.44	0.50
1:K:16:LEU:HD21	1:K:157:VAL:HG21	1.94	0.50
1:L:387:ALA:O	1:L:419:ARG:NH2	2.43	0.50
1:B:95:MET:HE3	1:C:307:ARG:HB3	1.94	0.50
1:L:423:ARG:HE	3:L:504:FBP:H12	1.77	0.49
1:C:370:GLU:O	1:C:431:ARG:NH2	2.42	0.49
1:C:46:HIS:NE2	2:C:502:SO4:O1	2.42	0.49
1:K:387:ALA:O	1:K:419:ARG:NH1	2.40	0.49
1:J:93:GLU:HG2	1:L:86:ARG:NE	2.27	0.49
1:B:13:ALA:O	1:B:17:PRO:HD2	2.13	0.49
1:F:171:PRO:HA	1:F:208:LYS:HE2	1.94	0.49
1:D:372:TRP:HB2	1:D:431:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:LEU:HD21	1:H:157:VAL:HG21	1.94	0.49
1:F:40:ARG:NH1	2:F:501:SO4:O2	2.46	0.48
1:I:431:ARG:OXT	1:I:431:ARG:HG3	2.13	0.48
1:I:46:HIS:HB3	1:I:351:PHE:CE2	2.49	0.48
1:G:419:ARG:NE	3:G:504:FBP:O4P	2.46	0.48
1:L:386:ARG:NH2	2:L:501:SO4:O4	2.46	0.48
1:B:44:ALA:O	1:B:52:ARG:NH1	2.45	0.48
1:P:44:ALA:O	1:P:52:ARG:NH1	2.45	0.48
1:D:418:THR:HG22	1:D:420:GLU:H	1.79	0.48
1:C:41:ALA:HB2	1:C:75:TYR:O	2.14	0.47
1:C:107:ARG:HB2	1:C:115:ARG:HD2	1.95	0.47
1:K:386:ARG:NH2	2:K:503:SO4:O4	2.48	0.47
1:E:40:ARG:NH2	1:E:385:ASP:OD1	2.47	0.47
1:G:44:ALA:O	1:G:52:ARG:NH1	2.40	0.47
1:E:126:ASP:OD1	1:E:126:ASP:N	2.48	0.47
1:H:237:SER:OG	1:H:243:ASP:OD2	2.23	0.47
1:D:406:ARG:HB3	1:D:425:LEU:HD21	1.95	0.47
1:I:307:ARG:NH1	1:L:94:GLU:OE2	2.47	0.47
1:N:23:LEU:HD21	1:N:128:ILE:HD13	1.97	0.47
1:E:237:SER:OG	1:E:243:ASP:OD2	2.23	0.47
1:H:44:ALA:O	1:H:52:ARG:NH1	2.45	0.47
1:B:16:LEU:HD11	1:B:157:VAL:HG21	1.96	0.46
1:L:41:ALA:HB2	1:L:75:TYR:O	2.16	0.46
1:L:16:LEU:HD21	1:L:157:VAL:HG21	1.98	0.46
1:G:201:SER:HB3	1:G:206:PRO:HA	1.97	0.46
1:A:46:HIS:HB3	1:A:351:PHE:CE2	2.51	0.45
1:E:387:ALA:O	1:E:419:ARG:NH1	2.43	0.45
1:B:93:GLU:HG2	1:D:86:ARG:NE	2.30	0.45
1:K:46:HIS:HB3	1:K:351:PHE:CE2	2.52	0.45
1:D:429:GLN:O	1:D:431:ARG:HB2	2.16	0.45
1:F:46:HIS:HB3	1:F:351:PHE:CE2	2.52	0.45
1:A:427:HIS:CD2	1:A:427:HIS:H	2.34	0.45
1:D:46:HIS:HB3	1:D:351:PHE:CE2	2.51	0.45
1:E:86:ARG:HB3	1:E:309:TYR:CD1	2.52	0.45
1:K:183:VAL:HG12	1:K:189:ILE:HA	1.98	0.45
1:F:44:ALA:O	1:F:52:ARG:NH1	2.44	0.45
1:L:46:HIS:HB3	1:L:351:PHE:CE2	2.52	0.45
1:A:233:ASP:HA	1:A:234:GLU:HA	1.64	0.45
1:B:10:LEU:HD22	1:B:10:LEU:H	1.82	0.45
1:F:387:ALA:O	1:F:419:ARG:HD3	2.16	0.44
1:L:201:SER:HB2	1:L:206:PRO:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ALA:O	1:C:52:ARG:NH1	2.48	0.44
1:D:396:ILE:HD13	1:D:417:VAL:HG21	1.99	0.44
1:G:389:VAL:H	1:G:429:GLN:HE21	1.65	0.44
1:H:46:HIS:HB3	1:H:351:PHE:CE2	2.52	0.44
1:K:370:GLU:O	1:K:431:ARG:NH1	2.45	0.44
1:L:40:ARG:NH2	1:L:385:ASP:OD1	2.51	0.44
1:D:386:ARG:NH1	2:D:503:SO4:O3	2.51	0.43
1:J:307:ARG:HB3	1:K:95:MET:HE3	2.00	0.43
1:B:14:ARG:NH2	1:C:63:ASN:O	2.51	0.43
1:G:46:HIS:HB3	1:G:351:PHE:CE2	2.53	0.43
1:I:430:GLU:O	1:I:431:ARG:HB3	2.17	0.43
1:F:40:ARG:NH2	1:F:385:ASP:OD1	2.51	0.43
1:B:95:MET:CE	1:C:307:ARG:HB3	2.49	0.43
1:C:186:ASN:O	1:C:187:ASP:HB2	2.18	0.43
1:F:20:SER:HA	1:F:135:TYR:O	2.19	0.43
1:N:46:HIS:HB3	1:N:351:PHE:CE2	2.53	0.43
1:C:42:LYS:HA	1:C:45:VAL:HG23	2.01	0.43
1:A:328:MET:SD	1:B:326:HIS:NE2	2.92	0.43
1:E:29:ARG:HG3	1:E:31:THR:HG23	2.01	0.43
1:L:418:THR:HG22	1:L:420:GLU:H	1.84	0.43
1:K:40:ARG:NE	2:K:503:SO4:O1	2.40	0.43
1:L:357:ASN:ND2	2:L:502:SO4:O4	2.52	0.43
1:A:40:ARG:NE	2:A:502:SO4:O3	2.51	0.42
1:P:321:ASP:OD2	1:P:325:SER:OG	2.37	0.42
1:I:40:ARG:NH2	1:I:385:ASP:OD1	2.52	0.42
1:C:201:SER:HB2	1:C:206:PRO:HA	2.01	0.42
1:B:46:HIS:HB3	1:B:351:PHE:CE2	2.55	0.42
1:C:16:LEU:HD21	1:C:157:VAL:HG21	2.01	0.42
1:F:14:ARG:HA	1:G:14:ARG:HG3	2.01	0.42
1:H:10:LEU:O	1:H:13:ALA:HB3	2.19	0.42
1:N:44:ALA:O	1:N:52:ARG:NH1	2.48	0.42
1:J:46:HIS:HB3	1:J:351:PHE:CE2	2.54	0.42
1:J:41:ALA:HB2	1:J:75:TYR:O	2.19	0.42
1:G:10:LEU:O	1:G:13:ALA:HB3	2.19	0.42
1:L:237:SER:OG	1:L:243:ASP:OD2	2.26	0.42
1:L:18:LEU:HA	1:L:18:LEU:HD13	1.90	0.42
1:L:14:ARG:NH1	1:L:18:LEU:HD21	2.35	0.42
1:C:326:HIS:CD2	1:D:330:LEU:HB2	2.55	0.42
1:H:339:VAL:HB	1:H:355:ARG:HD2	2.02	0.42
1:G:419:ARG:HH12	1:G:431:ARG:HD3	1.85	0.42
1:C:226:LEU:HD22	1:C:244:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:HIS:HB3	1:E:351:PHE:CE2	2.55	0.41
1:K:10:LEU:O	1:K:13:ALA:HB3	2.19	0.41
1:F:20:SER:HB3	1:F:135:TYR:HB2	2.02	0.41
1:E:330:LEU:HB3	1:E:346:VAL:HG22	2.02	0.41
1:A:428:LYS:HG3	1:A:430:GLU:H	1.85	0.41
1:B:347:GLN:O	1:B:364:SER:HA	2.21	0.41
1:C:86:ARG:HB3	1:C:309:TYR:CD1	2.54	0.41
1:J:201:SER:OG	1:J:206:PRO:HA	2.21	0.41
1:C:14:ARG:O	1:C:18:LEU:HD23	2.21	0.41
1:J:226:LEU:HD11	1:J:248:ILE:HG12	2.03	0.41
1:M:335:SER:HA	1:N:315:PRO:HB3	2.03	0.41
1:A:10:LEU:O	1:A:13:ALA:HB3	2.21	0.41
1:H:52:ARG:HD2	1:H:83:HIS:CG	2.56	0.41
1:J:307:ARG:NH1	1:K:94:GLU:OE1	2.54	0.41
1:F:357:ASN:ND2	1:F:373:VAL:O	2.47	0.40
1:L:72:ILE:HG21	1:L:120:ALA:HB1	2.03	0.40
1:C:52:ARG:HD2	1:C:83:HIS:CG	2.57	0.40
1:E:244:LEU:O	1:E:248:ILE:HG13	2.21	0.40
1:H:363:ASP:O	1:H:380:ARG:HA	2.21	0.40
1:P:347:GLN:O	1:P:364:SER:HA	2.20	0.40
1:C:339:VAL:HB	1:C:355:ARG:HD2	2.03	0.40
1:C:46:HIS:HB3	1:C:351:PHE:CE2	2.57	0.40
1:D:363:ASP:OD1	1:L:322:ARG:NH2	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLU:OE1	1:I:325:SER:OG[2_445]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/431 (94%)	387 (96%)	17 (4%)	1 (0%)	47	80
1	B	413/431 (96%)	397 (96%)	15 (4%)	1 (0%)	47	80
1	C	416/431 (96%)	403 (97%)	13 (3%)	0	100	100
1	D	394/431 (91%)	381 (97%)	13 (3%)	0	100	100
1	E	402/431 (93%)	388 (96%)	14 (4%)	0	100	100
1	F	394/431 (91%)	383 (97%)	11 (3%)	0	100	100
1	G	401/431 (93%)	391 (98%)	10 (2%)	0	100	100
1	H	402/431 (93%)	387 (96%)	14 (4%)	1 (0%)	47	80
1	I	403/431 (94%)	390 (97%)	13 (3%)	0	100	100
1	J	403/431 (94%)	392 (97%)	11 (3%)	0	100	100
1	K	401/431 (93%)	388 (97%)	13 (3%)	0	100	100
1	L	411/431 (95%)	396 (96%)	15 (4%)	0	100	100
1	M	221/431 (51%)	216 (98%)	5 (2%)	0	100	100
1	N	359/431 (83%)	348 (97%)	10 (3%)	1 (0%)	41	74
1	O	348/431 (81%)	338 (97%)	10 (3%)	0	100	100
1	P	327/431 (76%)	318 (97%)	9 (3%)	0	100	100
All	All	6100/6896 (88%)	5903 (97%)	193 (3%)	4 (0%)	51	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ASP
1	A	187	ASP
1	H	76	GLN
1	N	187	ASP

### 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	296/373 (79%)	291 (98%)	5 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	335/373 (90%)	327 (98%)	8 (2%)	49	78
1	C	352/373 (94%)	348 (99%)	4 (1%)	73	90
1	D	286/373 (77%)	281 (98%)	5 (2%)	60	84
1	E	322/373 (86%)	317 (98%)	5 (2%)	62	85
1	F	319/373 (86%)	315 (99%)	4 (1%)	69	88
1	G	331/373 (89%)	326 (98%)	5 (2%)	65	86
1	H	313/373 (84%)	307 (98%)	6 (2%)	57	82
1	I	330/373 (88%)	323 (98%)	7 (2%)	53	80
1	J	317/373 (85%)	311 (98%)	6 (2%)	57	82
1	K	324/373 (87%)	317 (98%)	7 (2%)	52	79
1	L	337/373 (90%)	330 (98%)	7 (2%)	53	80
1	M	19/373 (5%)	19 (100%)	0	100	100
1	N	150/373 (40%)	148 (99%)	2 (1%)	69	88
1	O	102/373 (27%)	102 (100%)	0	100	100
1	P	57/373 (15%)	57 (100%)	0	100	100
All	All	4190/5968 (70%)	4119 (98%)	71 (2%)	60	84

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	77	SER
1	A	226	LEU
1	A	230	ASP
1	A	427	HIS
1	B	10	LEU
1	B	16	LEU
1	B	35	ASP
1	B	77	SER
1	B	94	GLU
1	B	186	ASN
1	B	226	LEU
1	B	341	SER
1	C	35	ASP
1	C	40	ARG
1	C	187	ASP
1	C	226	LEU

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Mol	Chain	Res	Type
1	D	35	ASP
1	D	37	THR
1	D	77	SER
1	D	423	ARG
1	D	431	ARG
1	E	18	LEU
1	E	35	ASP
1	E	94	GLU
1	E	189	ILE
1	E	307	ARG
1	F	31	THR
1	F	94	GLU
1	F	208	LYS
1	F	418	THR
1	G	35	ASP
1	G	94	GLU
1	G	187	ASP
1	G	226	LEU
1	G	386	ARG
1	H	35	ASP
1	H	77	SER
1	H	94	GLU
1	H	190	ILE
1	H	372	TRP
1	H	386	ARG
1	I	29	ARG
1	I	35	ASP
1	I	94	GLU
1	I	187	ASP
1	I	307	ARG
1	I	386	ARG
1	I	431	ARG
1	J	35	ASP
1	J	94	GLU
1	J	181	MET
1	J	183	VAL
1	J	352	SER
1	J	430	GLU
1	K	10	LEU
1	K	35	ASP
1	K	181	MET
1	K	226	LEU

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Mol	Chain	Res	Type
1	K	329	THR
1	K	386	ARG
1	K	430	GLU
1	L	14	ARG
1	L	18	LEU
1	L	77	SER
1	L	173	GLU
1	L	307	ARG
1	L	311	GLU
1	L	386	ARG
1	N	68	ARG
1	N	418	THR

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

Mol	Chain	Res	Type
1	H	78	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

43 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	SO4	H	502	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	G	503	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	E	502	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.07	0
3	FBP	C	504	-	18,20,20	0.56	0	23,32,32	0.76	0
2	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	K	502	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	H	504	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	502	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	P	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	502	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	J	501	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	L	502	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	P	502	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	G	502	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	501	-	4,4,4	0.14	0	6,6,6	0.08	0
3	FBP	L	504	-	18,20,20	0.57	0	23,32,32	0.82	0
2	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	J	502	-	4,4,4	0.14	0	6,6,6	0.05	0
3	FBP	I	504	-	18,20,20	0.44	0	23,32,32	0.78	1 (4%)
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.07	0
3	FBP	G	504	-	18,20,20	0.43	0	23,32,32	0.80	1 (4%)
2	SO4	L	503	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	J	503	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	H	503	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	I	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	I	502	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	L	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	503	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	K	503	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	I	503	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	G	501	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	K	501	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	H	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	502	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.06	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
3	FBP	G	504	-	-	9/13/32/32	0/1/1/1
3	FBP	L	504	-	-	8/13/32/32	0/1/1/1
3	FBP	C	504	-	-	10/13/32/32	0/1/1/1
3	FBP	I	504	-	-	5/13/32/32	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	504	FBP	P2-O6-C6	2.22	124.42	118.30
3	I	504	FBP	P2-O6-C6	2.16	124.23	118.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	504	FBP	C1-O1-P1-O1P
3	C	504	FBP	C1-O1-P1-O2P
3	C	504	FBP	C1-O1-P1-O3P
3	C	504	FBP	C6-O6-P2-O4P
3	L	504	FBP	C1-O1-P1-O1P
3	L	504	FBP	O1-C1-C2-O2
3	L	504	FBP	O1-C1-C2-C3
3	L	504	FBP	O1-C1-C2-O5
3	I	504	FBP	O1-C1-C2-C3
3	I	504	FBP	C4-C5-C6-O6
3	I	504	FBP	C6-O6-P2-O5P
3	I	504	FBP	C6-O6-P2-O6P
3	G	504	FBP	C1-O1-P1-O1P
3	G	504	FBP	C1-O1-P1-O2P

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Mol	Chain	Res	Type	Atoms
3	G	504	FBP	C1-O1-P1-O3P
3	G	504	FBP	O1-C1-C2-C3
3	G	504	FBP	O1-C1-C2-O5
3	G	504	FBP	C6-O6-P2-O4P
3	G	504	FBP	C6-O6-P2-O5P
3	G	504	FBP	C6-O6-P2-O6P
3	C	504	FBP	C4-C5-C6-O6
3	C	504	FBP	O5-C5-C6-O6
3	L	504	FBP	C4-C5-C6-O6
3	L	504	FBP	O5-C5-C6-O6
3	I	504	FBP	O5-C5-C6-O6
3	C	504	FBP	C6-O6-P2-O5P
3	L	504	FBP	C6-O6-P2-O5P
3	C	504	FBP	C5-C6-O6-P2
3	L	504	FBP	C5-C6-O6-P2
3	G	504	FBP	O1-C1-C2-O2
3	C	504	FBP	O1-C1-C2-C3
3	C	504	FBP	C6-O6-P2-O6P

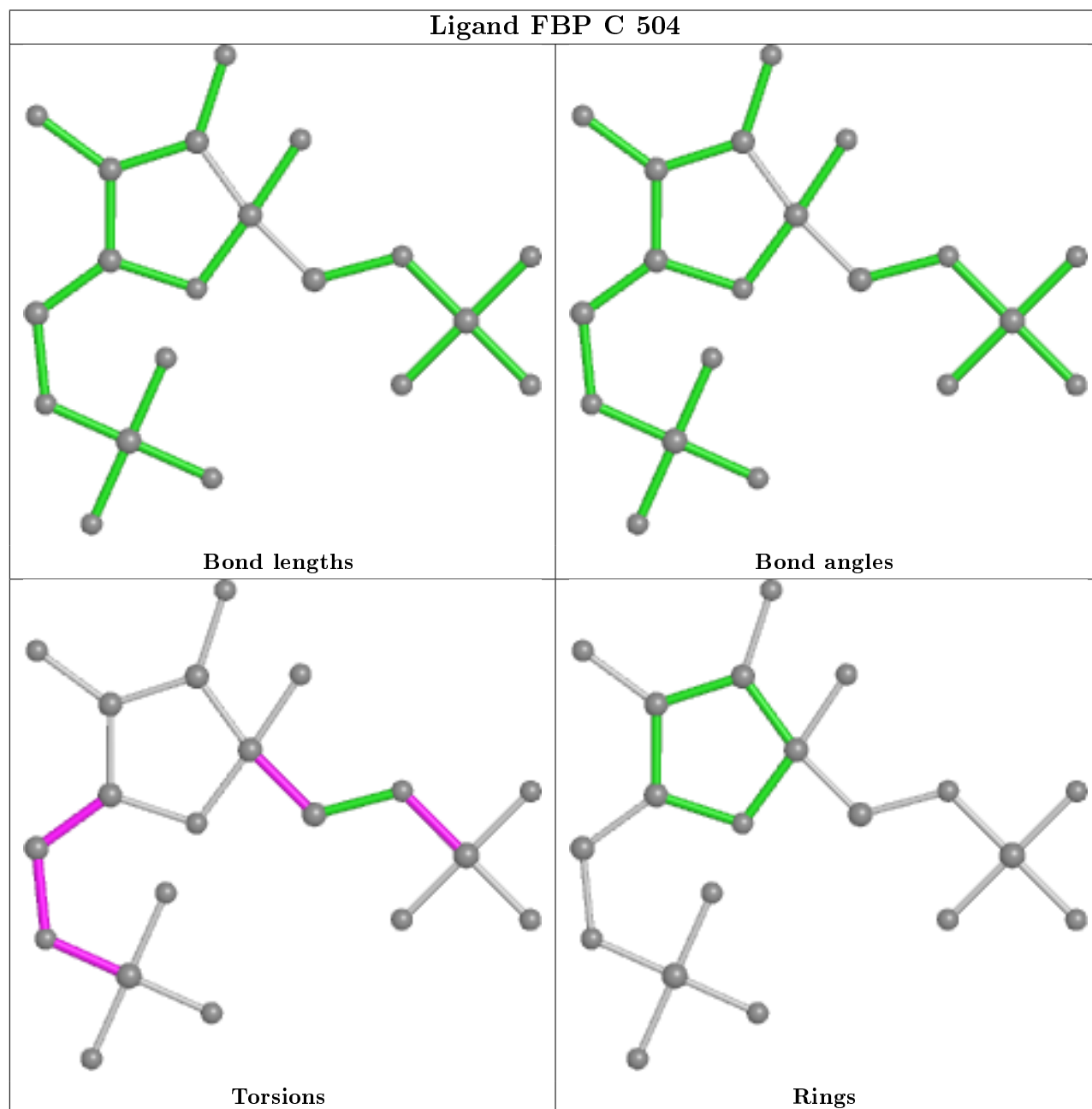
There are no ring outliers.

14 monomers are involved in 21 short contacts:

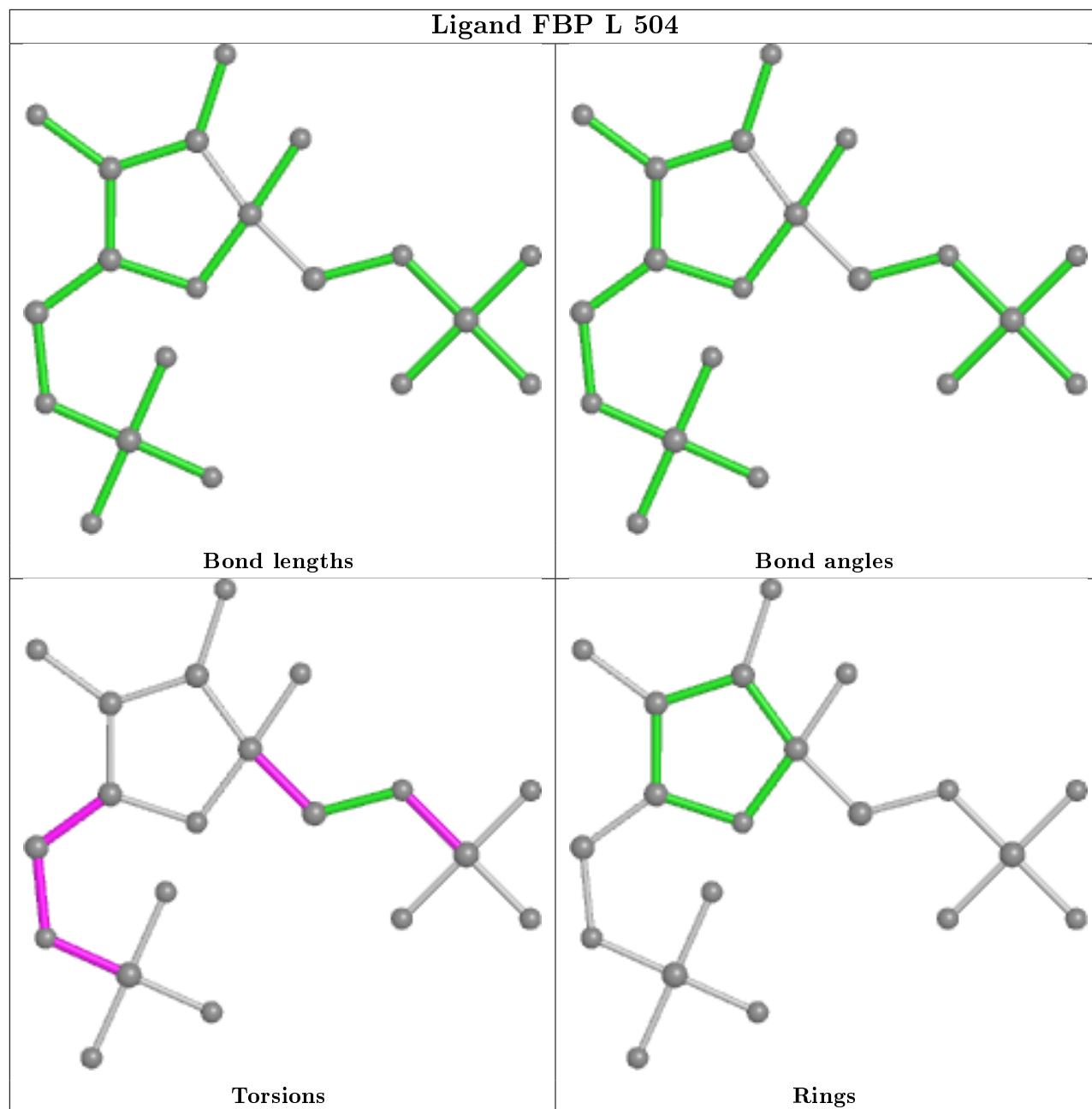
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	SO4	1	0
2	C	502	SO4	1	0
2	A	502	SO4	1	0
2	D	503	SO4	1	0
2	J	501	SO4	2	0
2	L	502	SO4	1	0
2	F	501	SO4	3	0
2	E	501	SO4	3	0
3	L	504	FBP	1	0
3	G	504	FBP	1	0
2	I	501	SO4	2	0
2	L	501	SO4	1	0
2	K	503	SO4	2	0
2	G	501	SO4	1	0

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

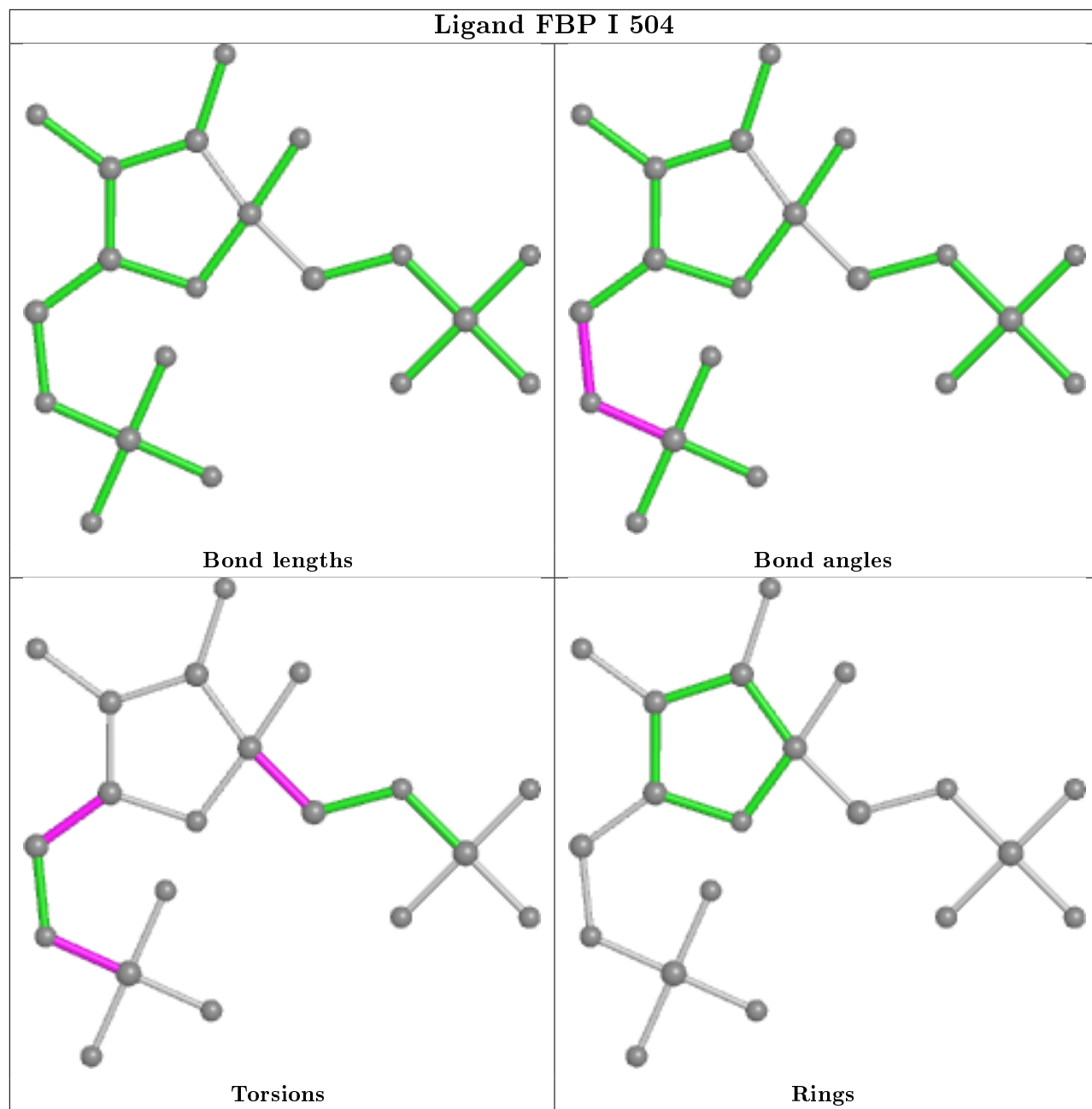
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

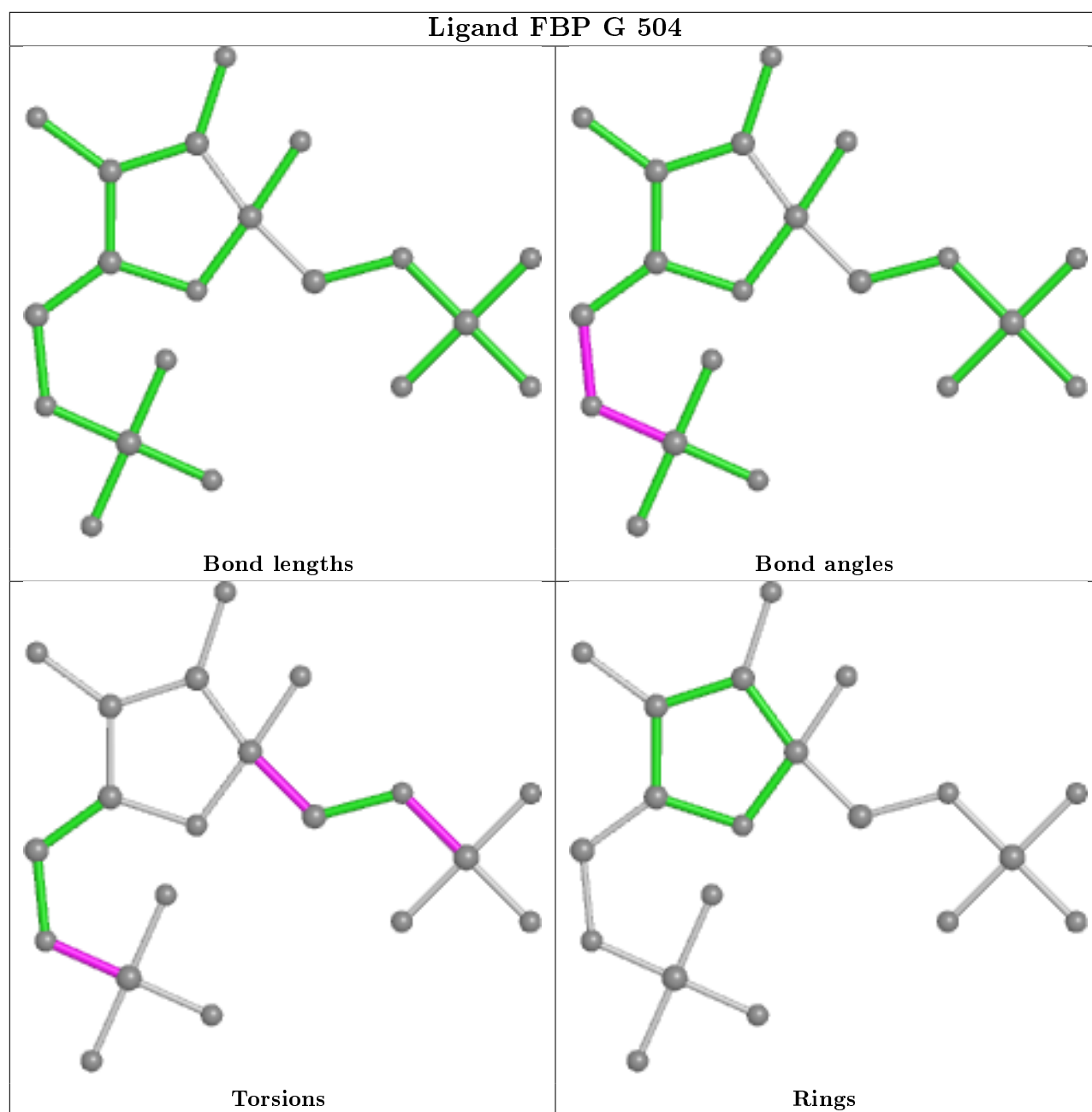


## Ligand FBP L 504



## Ligand FBP I 504





## 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	409/431 (94%)	0.04	12 (2%) 51 23	59, 96, 145, 179	0
1	B	417/431 (96%)	-0.25	2 (0%) 91 75	44, 78, 119, 152	0
1	C	418/431 (96%)	-0.34	1 (0%) 95 87	25, 53, 97, 129	0
1	D	402/431 (93%)	-0.03	13 (3%) 47 21	24, 75, 160, 187	0
1	E	408/431 (94%)	0.02	5 (1%) 79 53	39, 90, 166, 193	0
1	F	402/431 (93%)	0.04	8 (1%) 65 36	44, 84, 155, 187	0
1	G	409/431 (94%)	-0.26	0 100 100	35, 69, 113, 136	0
1	H	408/431 (94%)	0.02	7 (1%) 70 42	31, 84, 148, 180	0
1	I	409/431 (94%)	-0.20	0 100 100	36, 68, 113, 154	0
1	J	407/431 (94%)	0.14	19 (4%) 31 12	41, 88, 156, 179	0
1	K	409/431 (94%)	-0.09	8 (1%) 65 36	32, 78, 130, 170	0
1	L	415/431 (96%)	-0.21	4 (0%) 82 59	30, 67, 124, 168	0
1	M	229/431 (53%)	1.51	79 (34%) 0 0	120, 197, 256, 270	0
1	N	369/431 (85%)	0.78	66 (17%) 1 0	85, 153, 207, 239	0
1	O	364/431 (84%)	0.45	37 (10%) 6 2	70, 147, 196, 211	0
1	P	339/431 (78%)	0.49	38 (11%) 5 1	67, 141, 202, 244	0
All	All	6214/6896 (90%)	0.08	299 (4%) 30 11	24, 89, 186, 270	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	383	VAL	8.9
1	M	366	VAL	8.3
1	P	237	SER	7.6
1	M	143	HIS	6.6
1	M	374	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	O	391	PRO	6.4
1	M	382	CYS	6.3
1	M	145	TYR	6.2
1	M	391	PRO	6.1
1	J	255	TYR	6.1
1	O	390	ILE	5.9
1	M	416	LEU	5.9
1	N	255	TYR	5.5
1	N	297	LEU	5.5
1	N	147	GLN	5.5
1	M	398	GLU	5.4
1	N	272	PRO	5.3
1	P	141	GLY	5.3
1	N	390	ILE	5.3
1	N	254	ALA	5.2
1	M	384	ILE	5.2
1	N	153	LEU	5.2
1	N	144	ILE	5.1
1	M	415	VAL	5.1
1	O	253	LEU	5.1
1	M	414	ILE	5.0
1	J	253	LEU	5.0
1	M	365	ALA	5.0
1	O	167	CYS	5.0
1	N	316	ALA	5.0
1	O	196	PRO	4.9
1	J	254	ALA	4.9
1	M	399	ASN	4.9
1	N	256	ALA	4.7
1	J	267	ASP	4.6
1	N	382	CYS	4.6
1	N	374	GLY	4.6
1	J	256	ALA	4.4
1	O	35	ASP	4.3
1	P	65	GLY	4.3
1	M	385	ASP	4.2
1	O	197	ALA	4.2
1	M	390	ILE	4.2
1	O	211	ALA	4.2
1	N	348	SER	4.2
1	D	256	ALA	4.1
1	O	383	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	386	ARG	4.1
1	N	152	MET	4.0
1	E	209	SER	4.0
1	O	182	ALA	4.0
1	M	367	LEU	4.0
1	P	163	CYS	4.0
1	M	140	ALA	4.0
1	M	134	GLU	4.0
1	M	153	LEU	4.0
1	M	340	ILE	4.0
1	N	373	VAL	4.0
1	D	219	ASP	3.9
1	M	332	SER	3.9
1	N	393	GLY	3.9
1	M	329	THR	3.9
1	M	151	ARG	3.8
1	O	258	PRO	3.8
1	M	136	VAL	3.8
1	M	287	ASN	3.8
1	N	135	TYR	3.7
1	P	272	PRO	3.7
1	P	241	GLY	3.7
1	M	297	LEU	3.7
1	N	183	VAL	3.7
1	M	420	GLU	3.7
1	N	136	VAL	3.6
1	M	372	TRP	3.6
1	P	140	ALA	3.6
1	M	293	VAL	3.6
1	O	282	ALA	3.6
1	O	256	ALA	3.6
1	M	133	ALA	3.5
1	J	209	SER	3.5
1	M	305	PRO	3.5
1	P	177	ALA	3.5
1	O	349	VAL	3.5
1	M	348	SER	3.5
1	M	397	GLY	3.4
1	O	163	CYS	3.4
1	M	316	ALA	3.3
1	P	96	ASN	3.3
1	N	271	GLU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	350	LEU	3.3
1	N	150	SER	3.3
1	M	373	VAL	3.3
1	K	74	GLN	3.3
1	A	326	HIS	3.2
1	N	262	SER	3.2
1	O	382	CYS	3.2
1	N	381	ARG	3.2
1	J	249	THR	3.2
1	P	294	VAL	3.2
1	P	243	ASP	3.2
1	M	323	SER	3.2
1	M	349	VAL	3.2
1	M	320	GLN	3.1
1	N	340	ILE	3.1
1	A	181	MET	3.1
1	P	160	GLY	3.1
1	N	149	TYR	3.1
1	N	358	SER	3.1
1	M	333	LEU	3.1
1	P	227	LEU	3.1
1	P	242	LYS	3.1
1	O	166	ALA	3.1
1	O	218	PHE	3.0
1	P	120	ALA	3.0
1	M	96	ASN	3.0
1	N	394	MET	3.0
1	J	235	ASN	3.0
1	A	211	ALA	3.0
1	M	274	TRP	3.0
1	K	9	HIS	3.0
1	N	250	GLU	3.0
1	K	222	TYR	3.0
1	M	71	VAL	2.9
1	N	218	PHE	2.9
1	E	180	VAL	2.9
1	M	150	SER	2.9
1	O	176	SER	2.9
1	M	146	LYS	2.9
1	N	235	ASN	2.9
1	H	163	CYS	2.9
1	P	169	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	206	PRO	2.9
1	N	146	LYS	2.8
1	M	322	ARG	2.8
1	O	385	ASP	2.8
1	J	183	VAL	2.8
1	N	414	ILE	2.8
1	O	377	CYS	2.8
1	J	210	LEU	2.8
1	M	147	GLN	2.8
1	M	70	GLY	2.8
1	O	212	SER	2.8
1	E	255	TYR	2.8
1	N	226	LEU	2.8
1	D	254	ALA	2.8
1	M	364	SER	2.8
1	M	141	GLY	2.8
1	P	83	HIS	2.8
1	D	255	TYR	2.8
1	O	389	VAL	2.8
1	M	339	VAL	2.7
1	P	135	TYR	2.7
1	P	231	ASP	2.7
1	O	254	ALA	2.7
1	M	139	LEU	2.7
1	M	334	VAL	2.7
1	N	248	ILE	2.7
1	O	396	ILE	2.7
1	O	174	GLU	2.7
1	D	168	MET	2.7
1	N	267	ASP	2.7
1	P	246	PRO	2.7
1	P	236	SER	2.7
1	H	249	THR	2.7
1	N	397	GLY	2.7
1	K	249	THR	2.7
1	L	190	ILE	2.6
1	H	236	SER	2.6
1	A	210	LEU	2.6
1	H	192	PHE	2.6
1	O	183	VAL	2.6
1	N	396	ILE	2.6
1	H	250	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	326	HIS	2.6
1	F	105	GLN	2.6
1	M	387	ALA	2.6
1	N	376	SER	2.6
1	M	401	GLU	2.5
1	O	209	SER	2.5
1	P	95	MET	2.5
1	N	318	PHE	2.5
1	M	347	GLN	2.5
1	B	330	LEU	2.5
1	M	408	TYR	2.5
1	D	163	CYS	2.5
1	J	189	ILE	2.5
1	M	67	ARG	2.5
1	N	298	ASP	2.5
1	O	397	GLY	2.5
1	N	273	TYR	2.5
1	N	211	ALA	2.5
1	N	290	LEU	2.5
1	M	371	VAL	2.5
1	P	217	VAL	2.5
1	N	58	LEU	2.4
1	M	396	ILE	2.4
1	D	196	PRO	2.4
1	M	138	ILE	2.4
1	P	225	GLU	2.4
1	N	379	LEU	2.4
1	J	222	TYR	2.4
1	N	365	ALA	2.4
1	F	163	CYS	2.4
1	M	403	ASP	2.4
1	M	356	VAL	2.4
1	F	193	VAL	2.4
1	F	192	PHE	2.4
1	M	426	GLY	2.4
1	N	32	ARG	2.4
1	N	329	THR	2.4
1	D	241	GLY	2.4
1	M	325	SER	2.4
1	J	414	ILE	2.4
1	N	264	VAL	2.3
1	P	235	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	218	PHE	2.3
1	J	187	ASP	2.3
1	O	73	THR	2.3
1	P	239	ASP	2.3
1	H	161	ALA	2.3
1	P	297	LEU	2.3
1	O	326	HIS	2.3
1	A	165	VAL	2.3
1	L	116	GLY	2.3
1	E	173	GLU	2.3
1	E	197	ALA	2.3
1	L	221	ASP	2.3
1	M	135	TYR	2.3
1	N	47	PHE	2.3
1	A	203	PRO	2.3
1	N	332	SER	2.3
1	N	145	TYR	2.3
1	O	241	GLY	2.3
1	N	263	CYS	2.3
1	M	64	SER	2.3
1	C	113	TRP	2.3
1	F	240	PHE	2.3
1	P	122	THR	2.2
1	F	198	ASN	2.2
1	M	357	ASN	2.2
1	M	306	ILE	2.2
1	P	252	GLY	2.2
1	M	381	ARG	2.2
1	K	253	LEU	2.2
1	N	33	LEU	2.2
1	M	144	ILE	2.2
1	A	199	PRO	2.2
1	D	187	ASP	2.2
1	N	253	LEU	2.2
1	J	192	PHE	2.2
1	A	200	PRO	2.2
1	P	223	LEU	2.2
1	A	12	LEU	2.2
1	M	63	ASN	2.2
1	N	407	PHE	2.2
1	N	54	ILE	2.2
1	N	317	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	375	ARG	2.2
1	A	180	VAL	2.2
1	O	249	THR	2.2
1	J	180	VAL	2.1
1	N	426	GLY	2.1
1	P	49	GLY	2.1
1	P	338	CYS	2.1
1	N	417	VAL	2.1
1	K	13	ALA	2.1
1	P	300	TYR	2.1
1	J	211	ALA	2.1
1	A	198	ASN	2.1
1	J	163	CYS	2.1
1	M	317	LYS	2.1
1	O	36	LEU	2.1
1	O	405	ARG	2.1
1	F	255	TYR	2.1
1	P	211	ALA	2.1
1	F	253	LEU	2.1
1	N	36	LEU	2.1
1	K	183	VAL	2.1
1	J	168	MET	2.1
1	D	165	VAL	2.1
1	M	413	GLY	2.1
1	K	180	VAL	2.1
1	D	245	ILE	2.1
1	P	233	ASP	2.1
1	H	222	TYR	2.1
1	O	135	TYR	2.0
1	P	295	PRO	2.0
1	L	113	TRP	2.0
1	N	164	THR	2.0
1	P	116	GLY	2.0
1	N	265	GLN	2.0
1	M	283	TYR	2.0
1	N	323	SER	2.0
1	A	182	ALA	2.0
1	M	380	ARG	2.0
1	D	200	PRO	2.0
1	N	212	SER	2.0
1	B	329	THR	2.0
1	P	164	THR	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
3	FBP	I	504	20/20	0.77	0.24	79,138,171,209	0
2	SO4	J	503	5/5	0.80	0.17	117,132,142,157	0
3	FBP	L	504	20/20	0.82	0.30	81,139,188,189	0
3	FBP	G	504	20/20	0.83	0.29	72,152,203,206	0
2	SO4	P	502	5/5	0.86	0.21	79,82,137,151	0
3	FBP	C	504	20/20	0.89	0.21	67,122,166,185	0
2	SO4	A	503	5/5	0.89	0.26	95,124,132,170	0
2	SO4	K	503	5/5	0.91	0.19	73,89,109,110	0
2	SO4	D	504	5/5	0.92	0.23	77,84,97,116	0
2	SO4	A	501	5/5	0.93	0.12	92,101,111,132	0
2	SO4	I	502	5/5	0.93	0.17	69,80,89,98	0
2	SO4	I	503	5/5	0.93	0.15	66,66,117,120	0
2	SO4	K	501	5/5	0.93	0.08	112,117,131,144	0
2	SO4	F	501	5/5	0.94	0.16	77,78,105,111	0
2	SO4	E	503	5/5	0.94	0.15	96,97,118,122	0
2	SO4	B	502	5/5	0.94	0.12	75,97,117,126	0
2	SO4	H	501	5/5	0.94	0.12	74,95,102,105	0
2	SO4	P	501	5/5	0.95	0.10	66,92,123,145	0
2	SO4	B	501	5/5	0.95	0.09	102,128,135,146	0
2	SO4	D	502	5/5	0.95	0.13	83,105,110,111	0
2	SO4	L	503	5/5	0.95	0.16	77,79,96,100	0
2	SO4	F	502	5/5	0.95	0.11	67,68,94,100	0
2	SO4	G	502	5/5	0.96	0.10	79,79,104,106	0
2	SO4	D	503	5/5	0.96	0.15	60,80,95,96	0
2	SO4	B	503	5/5	0.96	0.19	69,81,88,100	0
2	SO4	J	502	5/5	0.97	0.09	67,71,96,129	0
2	SO4	K	502	5/5	0.97	0.11	62,73,85,93	0

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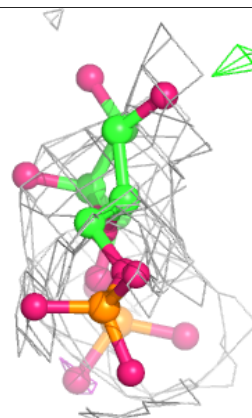
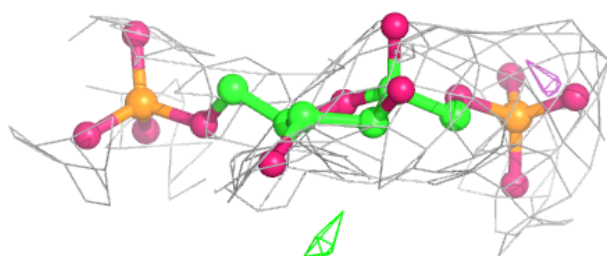
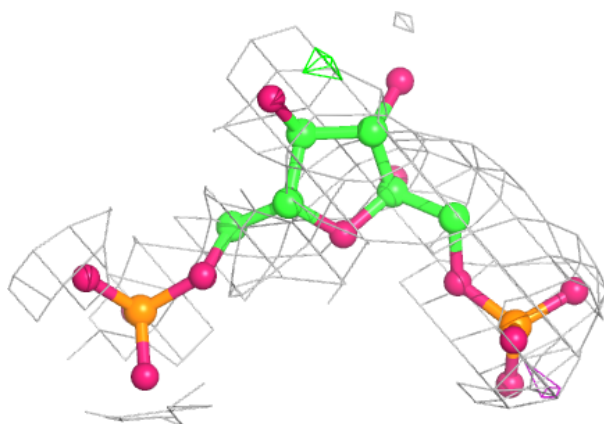
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	502	5/5	0.97	0.18	77,81,104,117	0
2	SO4	E	501	5/5	0.97	0.14	71,72,88,120	0
2	SO4	G	503	5/5	0.97	0.11	48,60,70,89	0
2	SO4	C	501	5/5	0.97	0.15	53,73,81,108	0
2	SO4	H	503	5/5	0.97	0.15	70,72,87,98	0
2	SO4	I	501	5/5	0.97	0.23	58,62,89,97	0
2	SO4	J	501	5/5	0.98	0.13	70,73,88,90	0
2	SO4	H	504	5/5	0.98	0.13	60,61,81,113	0
2	SO4	C	502	5/5	0.98	0.23	61,62,68,76	0
2	SO4	E	502	5/5	0.98	0.12	43,62,69,82	0
2	SO4	C	503	5/5	0.98	0.15	47,52,61,80	0
2	SO4	G	501	5/5	0.99	0.09	57,72,80,85	0
2	SO4	L	502	5/5	0.99	0.15	37,40,48,54	0
2	SO4	D	501	5/5	0.99	0.14	33,41,44,47	0
2	SO4	H	502	5/5	0.99	0.15	42,46,49,52	0
2	SO4	L	501	5/5	0.99	0.17	55,63,82,97	0

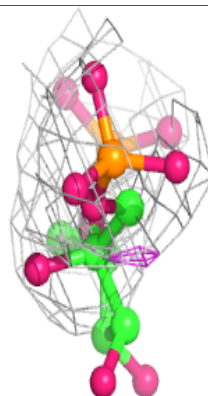
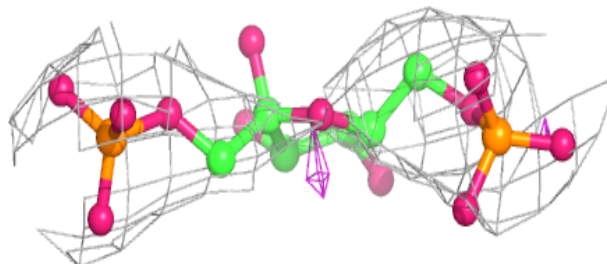
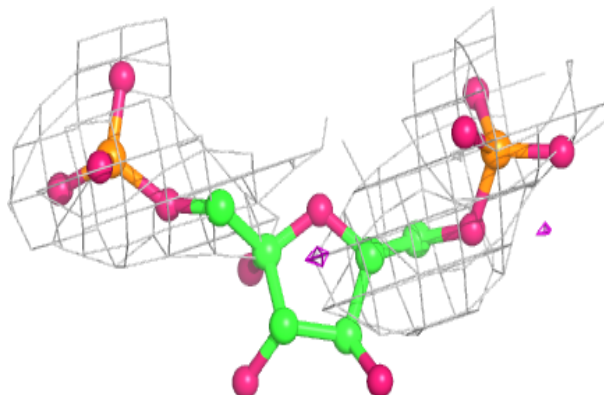
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FBP I 504:**

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

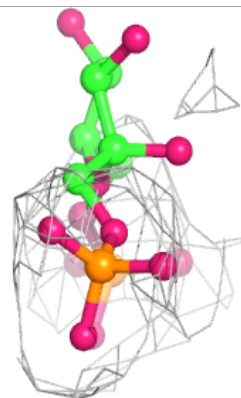
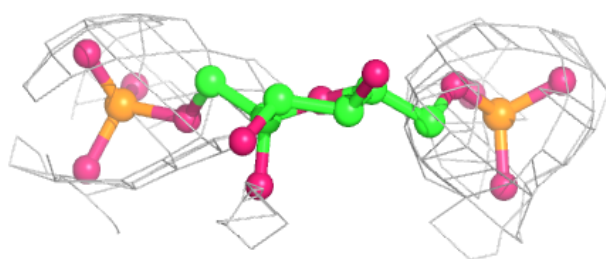
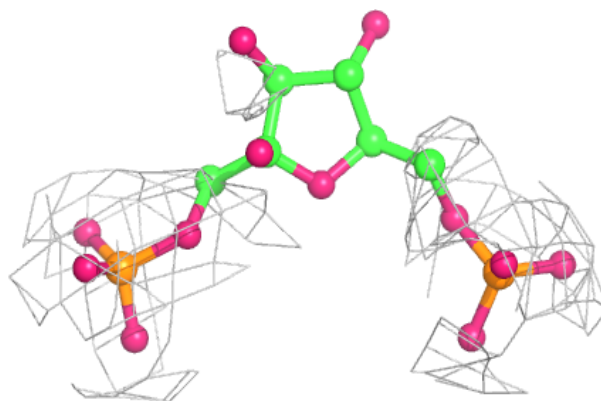
**Electron density around FBP L 504:**

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

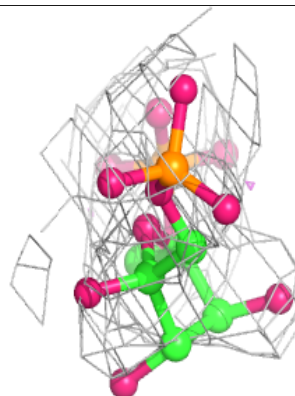
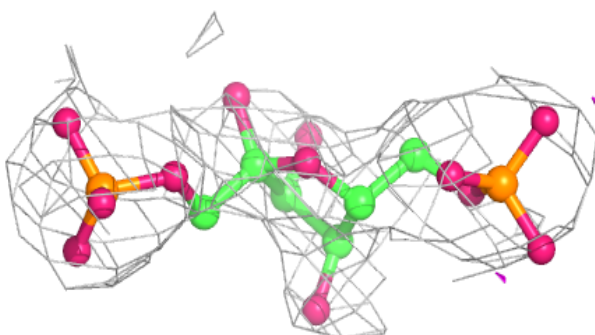
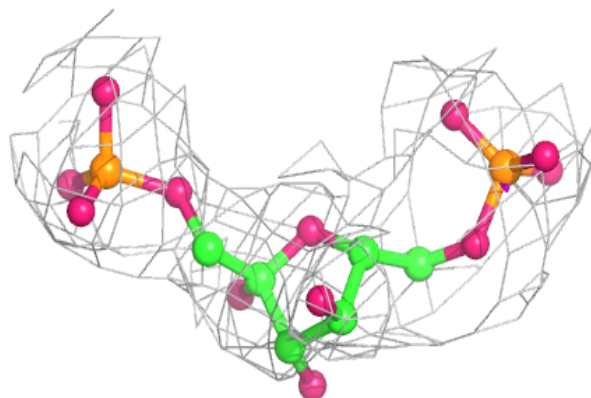


**Electron density around FBP G 504:**

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

**Electron density around FBP C 504:**

$2mF_o-DF_c$  (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.