



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 08:10 PM JST

PDB ID : 7E4S  
Title : Crystal structure of Lactobacillus rhamnosus 4-deoxy-L-threo-5-hexosulose-urionate ketol-isomerase KduI complexed with HEPES  
Authors : Yamamoto, Y.; Takase, R.; Mikami, B.; Hashimoto, W.  
Deposited on : 2021-02-15  
Resolution : 2.79 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.

---

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

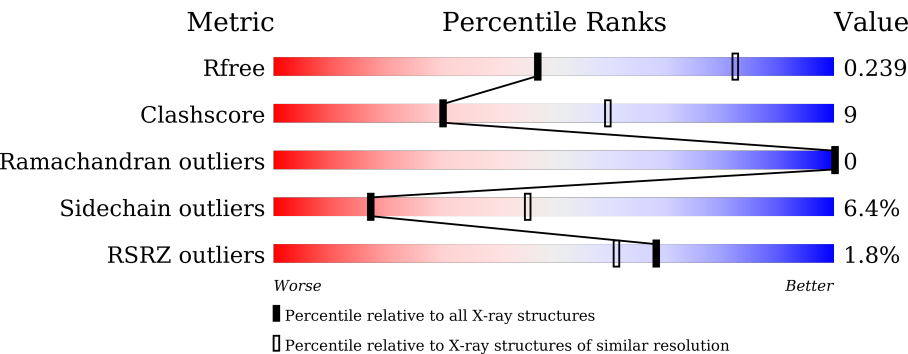
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

# 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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	289	<div><div>%</div><div><div></div><div>74%</div><div>21%</div><div></div><div></div></div><div></div></div>
1	B	289	<div><div>%</div><div><div></div><div>79%</div><div>17%</div><div></div><div></div></div><div></div></div>
1	C	289	<div><div>4%</div><div><div></div><div>72%</div><div>20%</div><div></div><div></div></div><div></div></div>
1	D	289	<div><div></div><div><div></div><div>71%</div><div>17%</div><div></div><div>10%</div></div><div></div></div>
1	E	289	<div><div>3%</div><div><div></div><div>69%</div><div>23%</div><div></div><div></div></div><div></div></div>
1	F	289	<div><div>%</div><div><div></div><div>72%</div><div>22%</div><div></div><div></div></div><div></div></div>

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	EPE	D	301	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13356 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 5-dehydro-4-deoxy-D-glucuronate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			
1	B	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			
1	C	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			
1	D	260	Total	C	N	O	S	0	0	0
			2089	1331	351	391	16			
1	E	270	Total	C	N	O	S	0	0	0
			2168	1378	366	407	17			
1	F	279	Total	C	N	O	S	0	0	0
			2243	1423	378	424	18			

There are 48 discrepancies between the modelled and reference sequences:

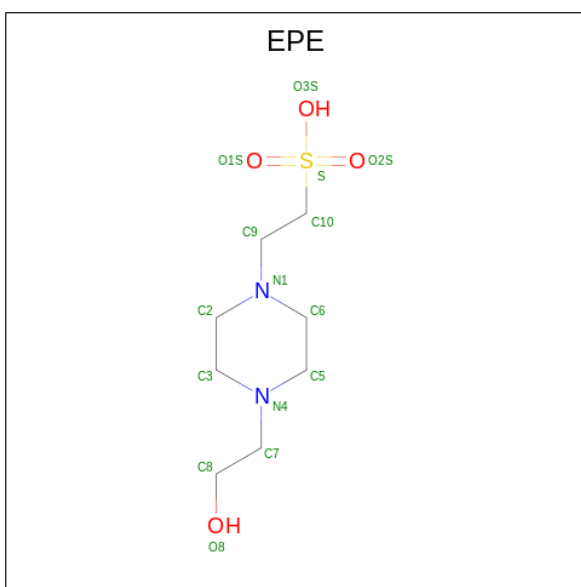
Chain	Residue	Modelled	Actual	Comment	Reference
A	282	LEU	-	expression tag	UNP A0A508YKK7
A	283	GLU	-	expression tag	UNP A0A508YKK7
A	284	HIS	-	expression tag	UNP A0A508YKK7
A	285	HIS	-	expression tag	UNP A0A508YKK7
A	286	HIS	-	expression tag	UNP A0A508YKK7
A	287	HIS	-	expression tag	UNP A0A508YKK7
A	288	HIS	-	expression tag	UNP A0A508YKK7
A	289	HIS	-	expression tag	UNP A0A508YKK7
B	282	LEU	-	expression tag	UNP A0A508YKK7
B	283	GLU	-	expression tag	UNP A0A508YKK7
B	284	HIS	-	expression tag	UNP A0A508YKK7
B	285	HIS	-	expression tag	UNP A0A508YKK7
B	286	HIS	-	expression tag	UNP A0A508YKK7
B	287	HIS	-	expression tag	UNP A0A508YKK7
B	288	HIS	-	expression tag	UNP A0A508YKK7
B	289	HIS	-	expression tag	UNP A0A508YKK7
C	282	LEU	-	expression tag	UNP A0A508YKK7

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	283	GLU	-	expression tag	UNP A0A508YKK7
C	284	HIS	-	expression tag	UNP A0A508YKK7
C	285	HIS	-	expression tag	UNP A0A508YKK7
C	286	HIS	-	expression tag	UNP A0A508YKK7
C	287	HIS	-	expression tag	UNP A0A508YKK7
C	288	HIS	-	expression tag	UNP A0A508YKK7
C	289	HIS	-	expression tag	UNP A0A508YKK7
D	282	LEU	-	expression tag	UNP A0A508YKK7
D	283	GLU	-	expression tag	UNP A0A508YKK7
D	284	HIS	-	expression tag	UNP A0A508YKK7
D	285	HIS	-	expression tag	UNP A0A508YKK7
D	286	HIS	-	expression tag	UNP A0A508YKK7
D	287	HIS	-	expression tag	UNP A0A508YKK7
D	288	HIS	-	expression tag	UNP A0A508YKK7
D	289	HIS	-	expression tag	UNP A0A508YKK7
E	282	LEU	-	expression tag	UNP A0A508YKK7
E	283	GLU	-	expression tag	UNP A0A508YKK7
E	284	HIS	-	expression tag	UNP A0A508YKK7
E	285	HIS	-	expression tag	UNP A0A508YKK7
E	286	HIS	-	expression tag	UNP A0A508YKK7
E	287	HIS	-	expression tag	UNP A0A508YKK7
E	288	HIS	-	expression tag	UNP A0A508YKK7
E	289	HIS	-	expression tag	UNP A0A508YKK7
F	282	LEU	-	expression tag	UNP A0A508YKK7
F	283	GLU	-	expression tag	UNP A0A508YKK7
F	284	HIS	-	expression tag	UNP A0A508YKK7
F	285	HIS	-	expression tag	UNP A0A508YKK7
F	286	HIS	-	expression tag	UNP A0A508YKK7
F	287	HIS	-	expression tag	UNP A0A508YKK7
F	288	HIS	-	expression tag	UNP A0A508YKK7
F	289	HIS	-	expression tag	UNP A0A508YKK7

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

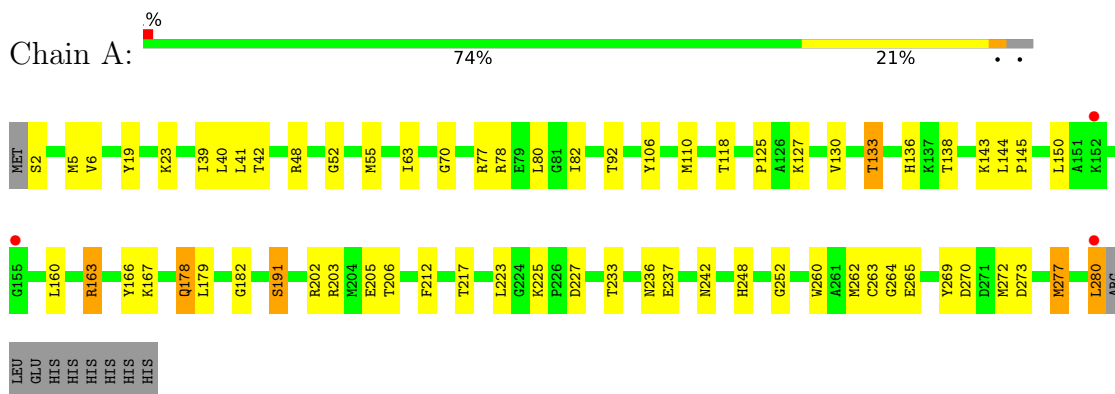
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	B	9	Total 9	O 9	0	0
4	C	4	Total 4	O 4	0	0
4	D	5	Total 5	O 5	0	0
4	E	5	Total 5	O 5	0	0
4	F	4	Total 4	O 4	0	0

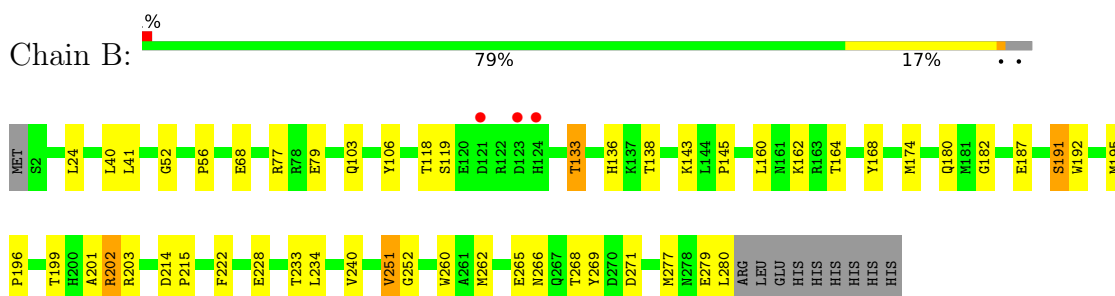
### 3 Residue-property plots [i](#)

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.

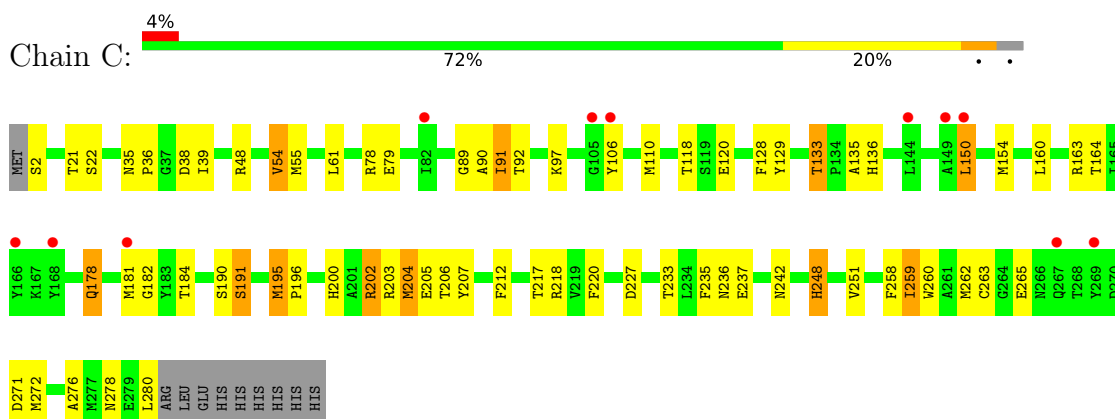
- Molecule 1: 5-dehydro-4-deoxy-D-glucuronate isomerase



- Molecule 1: 5-dehydro-4-deoxy-D-glucuronate isomerase

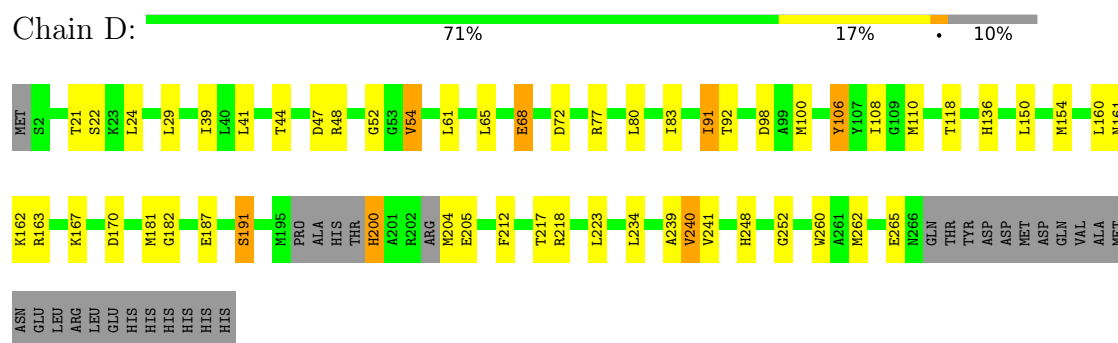


- Molecule 1: 5-dehydro-4-deoxy-D-glucuronate isomerase

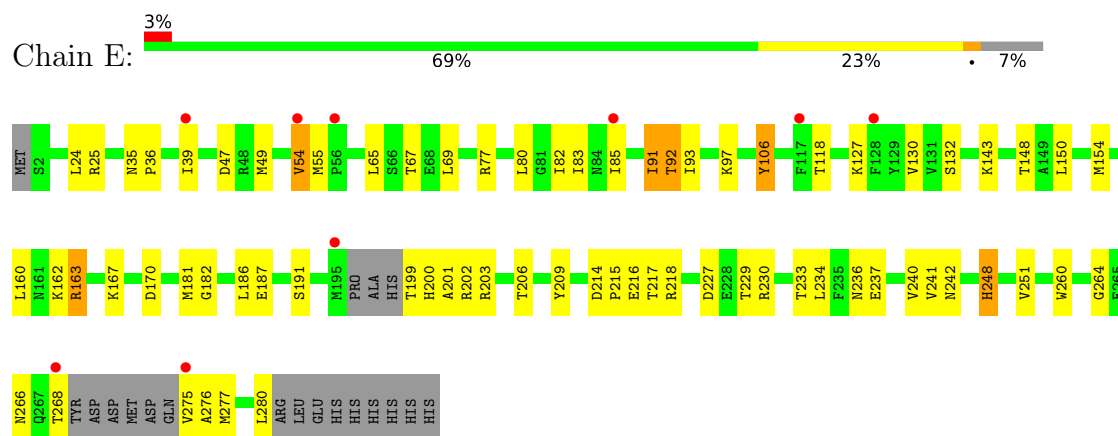




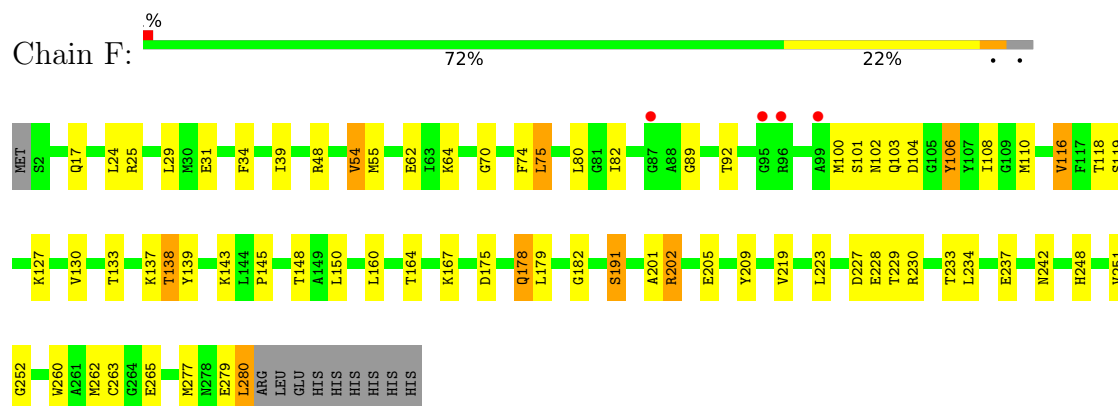
• Molecule 1: 5-dehydro-4-deoxy-D-glucuronate isomerase



• Molecule 1: 5-dehydro-4-deoxy-D-glucuronate isomerase



• Molecule 1: 5-dehydro-4-deoxy-D-glucuronate isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.29Å 189.25Å 117.80Å 90.00° 106.24° 90.00°	Depositor
Resolution (Å)	47.31 – 2.79 47.31 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.31-2.79) 98.0 (47.31-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, $R_{free}$	0.165 , 0.238 0.171 , 0.239	Depositor DCC
$R_{free}$ test set	2403 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.0	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13356	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: ZN, EPE

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	0.43	0/2303	0.66	0/3121
1	B	0.44	0/2303	0.65	0/3121
1	C	0.40	0/2303	0.64	0/3121
1	D	0.45	0/2144	0.66	0/2901
1	E	0.43	0/2223	0.64	0/3008
1	F	0.42	0/2303	0.66	0/3121
All	All	0.43	0/13579	0.65	0/18393

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2243	0	2144	45	0
1	B	2243	0	2144	34	0
1	C	2243	0	2144	49	0
1	D	2089	0	2004	39	0
1	E	2168	0	2085	46	0
1	F	2243	0	2144	53	0
2	A	15	0	17	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	17	1	0
2	C	15	0	17	0	0
2	D	15	0	17	1	0
2	E	15	0	17	0	0
2	F	15	0	17	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	4	0	0	0	0
4	B	9	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	4	0	0	0	0
All	All	13356	0	12767	243	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 9.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LEU:HD23	1:F:160:LEU:HD23	1.55	0.86
1:F:229:THR:H	1:F:280:LEU:HD21	1.46	0.80
1:A:160:LEU:HD23	1:E:160:LEU:HD23	1.65	0.78
1:F:262:MET:HE1	2:F:301:EPE:H71	1.69	0.74
1:C:54:VAL:HG22	1:C:128:PHE:HB2	1.70	0.74
1:C:195:MET:SD	1:C:195:MET:N	2.61	0.73
1:C:79:GLU:HG3	1:C:135:ALA:HB2	1.70	0.72
1:A:163:ARG:NH1	2:A:301:EPE:O3S	2.24	0.70
1:B:277:MET:O	1:C:218:ARG:HD2	1.92	0.69
1:C:203:ARG:HH11	1:C:271:ASP:HB3	1.56	0.68
1:A:39:ILE:HD13	1:A:63:ILE:HD13	1.74	0.68
1:C:92:THR:HG22	1:C:97:LYS:HG3	1.75	0.68
1:C:178:GLN:HG3	1:C:263:CYS:HB2	1.75	0.67
1:A:6:VAL:HG22	1:A:42:THR:HG22	1.77	0.66
1:E:25:ARG:NH2	1:E:233:THR:O	2.29	0.66
1:A:178:GLN:HG3	1:A:264:GLY:H	1.61	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:LEU:HD21	1:F:167:LYS:HB2	1.79	0.65
1:A:182:GLY:HA3	1:A:260:TRP:CZ2	2.32	0.65
1:A:127:LYS:NZ	1:A:237:GLU:OE2	2.27	0.65
1:A:178:GLN:HG3	1:A:264:GLY:O	1.98	0.64
1:E:150:LEU:HD21	1:E:167:LYS:HB2	1.79	0.62
1:D:65:LEU:HD22	1:D:68:GLU:HG3	1.79	0.62
1:A:277:MET:HG2	1:E:216:GLU:O	2.00	0.62
1:C:48:ARG:NH1	1:D:47:ASP:OD2	2.33	0.61
1:A:178:GLN:HG2	1:A:263:CYS:HB2	1.83	0.61
1:C:265:GLU:O	1:D:77:ARG:HD3	2.00	0.61
1:A:150:LEU:HD21	1:A:167:LYS:HB2	1.81	0.61
1:B:203:ARG:NH1	1:B:262:MET:SD	2.74	0.60
1:F:100:MET:HE1	1:F:106:TYR:HB2	1.84	0.59
1:B:192:TRP:CD2	1:B:251:VAL:HG13	2.37	0.59
1:C:204:MET:HE1	1:C:263:CYS:SG	2.43	0.59
1:E:242:ASN:OD1	1:E:248:HIS:HB3	2.02	0.59
1:A:212:PHE:HB3	1:A:217:THR:HB	1.84	0.59
1:E:201:ALA:HB3	1:E:202:ARG:NH1	2.18	0.58
1:A:205:GLU:OE2	2:A:301:EPE:H72	2.04	0.58
1:B:182:GLY:HA3	1:B:260:TRP:CZ2	2.38	0.58
1:C:129:TYR:HE2	1:C:259:ILE:HD11	1.67	0.58
1:A:110:MET:HE1	1:A:136:HIS:C	2.24	0.58
1:B:79:GLU:HG2	1:B:133:THR:HG22	1.83	0.58
1:A:191:SER:HG	1:A:252:GLY:H	1.51	0.58
1:E:229:THR:OG1	1:E:280:LEU:HD11	2.03	0.58
1:C:154:MET:HE2	1:C:163:ARG:NH1	2.19	0.57
1:C:90:ALA:O	1:C:118:THR:HG22	2.05	0.57
1:F:25:ARG:NH1	1:F:31:GLU:OE1	2.37	0.57
1:E:167:LYS:HD3	1:E:170:ASP:OD2	2.05	0.57
1:F:39:ILE:HG12	1:F:54:VAL:HB	1.87	0.56
1:E:82:ILE:HG12	1:E:130:VAL:HG12	1.88	0.56
1:F:178:GLN:HG3	1:F:263:CYS:HB2	1.87	0.56
1:F:229:THR:N	1:F:280:LEU:HD21	2.17	0.56
1:D:191:SER:HG	1:D:252:GLY:H	1.52	0.56
1:D:205:GLU:HG2	1:D:262:MET:HG3	1.87	0.56
1:C:79:GLU:HB2	1:C:133:THR:HG22	1.88	0.56
1:B:201:ALA:HB3	1:B:202:ARG:NH1	2.21	0.56
1:E:182:GLY:HA3	1:E:260:TRP:CZ2	2.41	0.55
1:E:199:THR:N	4:E:401:HOH:O	2.39	0.55
1:A:136:HIS:HB2	1:B:136:HIS:HB2	1.87	0.55
1:F:191:SER:O	1:F:191:SER:OG	2.23	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HG2	1:A:178:GLN:O	2.05	0.54
1:B:203:ARG:NH2	1:B:271:ASP:O	2.40	0.54
1:C:203:ARG:HD2	1:C:262:MET:SD	2.47	0.54
1:D:41:LEU:HD23	1:D:52:GLY:HA3	1.88	0.54
1:F:110:MET:O	1:F:138:THR:OG1	2.25	0.54
1:D:100:MET:HE1	1:D:106:TYR:HB2	1.89	0.54
1:F:17:GLN:O	1:F:230:ARG:NH1	2.41	0.54
1:C:136:HIS:HB2	1:D:136:HIS:HB2	1.89	0.54
1:D:205:GLU:OE2	2:D:301:EPE:H51	2.08	0.54
1:A:242:ASN:ND2	1:A:248:HIS:HB3	2.23	0.54
1:A:265:GLU:O	1:B:77:ARG:HD3	2.08	0.53
1:E:227:ASP:HA	1:E:280:LEU:H	1.73	0.53
1:C:78:ARG:NE	1:D:265:GLU:OE2	2.33	0.53
1:E:275:VAL:HG22	1:E:276:ALA:H	1.73	0.53
1:D:191:SER:OG	1:D:252:GLY:N	2.25	0.53
1:F:101:SER:N	1:F:104:ASP:OD2	2.41	0.52
1:F:191:SER:OG	1:F:252:GLY:N	2.34	0.52
1:A:82:ILE:HD12	1:A:130:VAL:HG12	1.90	0.52
1:A:269:TYR:HE2	2:A:301:EPE:H31	1.74	0.52
1:C:202:ARG:HG2	1:C:271:ASP:OD2	2.09	0.52
1:A:203:ARG:HB2	1:A:263:CYS:O	2.10	0.51
1:C:91:ILE:O	1:C:91:ILE:HG13	2.10	0.51
1:E:266:ASN:ND2	1:F:70:GLY:HA3	2.26	0.51
1:E:39:ILE:HG12	1:E:54:VAL:HB	1.91	0.51
1:E:202:ARG:HD2	1:E:202:ARG:N	2.25	0.51
1:F:102:ASN:OD1	1:F:103:GLN:HG2	2.10	0.51
1:F:227:ASP:HA	1:F:280:LEU:H	1.75	0.51
1:F:34:PHE:HB3	1:F:55:MET:HE2	1.92	0.51
1:D:182:GLY:HA3	1:D:260:TRP:CZ2	2.46	0.51
1:D:218:ARG:HD2	1:F:277:MET:O	2.11	0.51
1:E:85:ILE:HG13	1:E:127:LYS:HE3	1.93	0.51
1:A:133:THR:HG21	1:A:178:GLN:O	2.11	0.50
1:B:143:LYS:O	1:B:145:PRO:HD3	2.11	0.50
1:C:36:PRO:N	1:C:55:MET:HE3	2.26	0.50
1:C:39:ILE:HG12	1:C:54:VAL:HB	1.94	0.50
1:C:89:GLY:HA2	1:C:120:GLU:HG3	1.94	0.50
1:D:162:LYS:HG2	1:D:187:GLU:HG3	1.93	0.49
1:C:154:MET:HE2	1:C:163:ARG:HH12	1.76	0.49
1:A:143:LYS:O	1:A:145:PRO:HD3	2.12	0.49
1:A:202:ARG:HD2	1:A:202:ARG:N	2.28	0.49
1:B:41:LEU:HD23	1:B:52:GLY:HA3	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HD23	1:C:160:LEU:HD23	1.93	0.49
1:B:191:SER:OG	1:B:252:GLY:N	2.36	0.49
1:D:65:LEU:CD2	1:D:68:GLU:HG3	2.41	0.49
1:F:82:ILE:HD12	1:F:130:VAL:HG12	1.93	0.49
1:D:68:GLU:OE1	1:D:68:GLU:N	2.37	0.49
1:E:200:HIS:ND1	1:E:200:HIS:O	2.44	0.49
1:E:214:ASP:HB2	1:E:215:PRO:HD2	1.94	0.49
1:F:242:ASN:CG	1:F:248:HIS:HB3	2.33	0.49
1:E:69:LEU:HA	1:F:202:ARG:HD3	1.94	0.49
1:B:79:GLU:CG	1:B:133:THR:HG22	2.43	0.48
1:C:212:PHE:HB3	1:C:217:THR:HB	1.94	0.48
1:A:48:ARG:O	1:A:78:ARG:NH1	2.46	0.48
1:D:83:ILE:HG13	1:D:181:MET:HE1	1.96	0.48
1:E:80:LEU:HD13	1:E:132:SER:HB2	1.95	0.48
1:E:186:LEU:HD22	1:E:191:SER:HA	1.95	0.48
1:F:92:THR:HB	1:F:116:VAL:HG13	1.95	0.48
1:D:200:HIS:HE1	1:D:204:MET:HA	1.78	0.47
1:A:41:LEU:HD23	1:A:52:GLY:HA3	1.95	0.47
1:D:212:PHE:HB3	1:D:217:THR:HB	1.96	0.47
1:D:150:LEU:HD12	1:D:150:LEU:O	2.14	0.47
1:F:127:LYS:NZ	1:F:237:GLU:OE2	2.45	0.47
1:E:92:THR:HB	1:E:97:LYS:HA	1.96	0.46
1:B:201:ALA:HB3	1:B:202:ARG:HH11	1.78	0.46
1:A:80:LEU:HD21	1:A:82:ILE:HD11	1.96	0.46
1:B:162:LYS:HG2	1:B:187:GLU:HG3	1.98	0.46
1:D:39:ILE:HG12	1:D:54:VAL:HB	1.96	0.46
1:E:181:MET:HE3	1:E:181:MET:HB3	1.80	0.46
1:C:182:GLY:HA3	1:C:260:TRP:CZ2	2.50	0.46
1:D:21:THR:HG23	1:F:230:ARG:HH22	1.81	0.46
1:F:133:THR:HG21	1:F:179:LEU:HB2	1.97	0.46
1:E:47:ASP:OD2	1:F:48:ARG:NH1	2.49	0.46
1:F:25:ARG:O	1:F:29:LEU:HB3	2.16	0.46
1:F:89:GLY:HA2	1:F:119:SER:HA	1.97	0.46
1:E:182:GLY:HA3	1:E:260:TRP:CE2	2.51	0.46
1:C:276:ALA:O	1:C:278:ASN:N	2.48	0.45
1:D:29:LEU:HD12	1:D:239:ALA:O	2.16	0.45
1:C:39:ILE:HD11	1:C:61:LEU:HB3	1.98	0.45
1:C:195:MET:H	1:C:195:MET:CE	2.29	0.45
1:C:203:ARG:NH1	1:C:271:ASP:HB3	2.28	0.45
1:A:262:MET:HE1	2:A:301:EPE:H81	1.98	0.45
1:B:40:LEU:O	1:B:52:GLY:HA3	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLU:HG3	1:C:135:ALA:CB	2.44	0.45
1:C:150:LEU:H	1:C:150:LEU:HG	1.59	0.45
1:E:83:ILE:HG13	1:E:181:MET:HE1	1.97	0.45
1:C:191:SER:O	1:C:251:VAL:HG23	2.17	0.45
1:E:91:ILE:HD11	1:E:106:TYR:CD2	2.52	0.45
1:F:110:MET:HB3	1:F:110:MET:HE2	1.68	0.45
1:F:150:LEU:H	1:F:150:LEU:HD23	1.81	0.45
1:A:77:ARG:HD3	1:B:265:GLU:O	2.16	0.45
1:A:150:LEU:H	1:A:150:LEU:HD23	1.82	0.45
1:F:191:SER:O	1:F:251:VAL:HA	2.17	0.45
1:B:234:LEU:HD21	1:B:240:VAL:HG23	1.99	0.45
1:F:80:LEU:HB3	1:F:108:ILE:HB	1.98	0.45
1:F:148:THR:O	1:F:148:THR:HG22	2.17	0.45
1:A:82:ILE:CD1	1:A:130:VAL:HG12	2.47	0.44
1:B:56:PRO:HG2	1:B:119:SER:OG	2.16	0.44
1:F:201:ALA:C	1:F:202:ARG:HE	2.20	0.44
1:F:205:GLU:OE2	2:F:301:EPE:H52	2.17	0.44
1:C:242:ASN:OD1	1:C:248:HIS:HB3	2.17	0.44
1:D:161:ASN:O	1:D:163:ARG:HD3	2.16	0.44
1:C:2:SER:HB2	1:C:38:ASP:OD1	2.17	0.44
1:D:110:MET:HB3	1:D:110:MET:HE2	1.68	0.44
1:B:234:LEU:HD21	1:B:240:VAL:CG2	2.48	0.44
1:F:62:GLU:HG3	1:F:64:LYS:HG3	1.98	0.44
1:A:55:MET:HE2	1:A:125:PRO:HG2	1.98	0.44
1:D:44:THR:O	1:D:48:ARG:HA	2.18	0.44
1:E:35:ASN:OD1	1:E:36:PRO:HD2	2.18	0.44
1:E:36:PRO:N	1:E:55:MET:HE3	2.33	0.44
1:F:182:GLY:HA3	1:F:260:TRP:CZ2	2.53	0.44
1:D:21:THR:HG23	1:F:230:ARG:NH2	2.32	0.44
1:C:181:MET:HE3	1:C:181:MET:HB3	1.75	0.44
1:F:137:LYS:HD2	1:F:139:TYR:CZ	2.53	0.44
1:C:39:ILE:HG13	1:C:61:LEU:HD13	2.00	0.44
1:E:91:ILE:HD12	1:E:93:ILE:HD11	1.99	0.44
1:F:24:LEU:HD23	1:F:24:LEU:HA	1.70	0.44
1:F:209:TYR:CD1	1:F:234:LEU:HD12	2.53	0.44
1:A:70:GLY:HA3	1:B:266:ASN:ND2	2.33	0.43
1:E:203:ARG:HA	1:E:264:GLY:HA3	2.00	0.43
1:F:150:LEU:CD2	1:F:167:LYS:HB2	2.47	0.43
1:A:182:GLY:HA3	1:A:260:TRP:CE2	2.53	0.43
1:B:260:TRP:CD2	2:B:301:EPE:H62	2.53	0.43
1:D:39:ILE:HD11	1:D:61:LEU:HB3	1.99	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ILE:HG13	1:E:181:MET:CE	2.47	0.43
1:B:214:ASP:HB2	1:B:215:PRO:HD2	1.99	0.43
1:E:77:ARG:HD3	1:F:265:GLU:O	2.17	0.43
1:F:229:THR:OG1	1:F:280:LEU:HD21	2.19	0.43
2:F:301:EPE:H102	2:F:301:EPE:H22	1.71	0.43
1:D:182:GLY:HA3	1:D:260:TRP:CE2	2.53	0.43
1:C:35:ASN:OD1	1:C:36:PRO:HD2	2.18	0.43
1:C:204:MET:HB3	1:C:204:MET:HE2	1.48	0.43
1:A:5:MET:HA	1:A:41:LEU:O	2.18	0.43
1:A:191:SER:OG	1:A:252:GLY:N	2.31	0.43
1:E:209:TYR:CD1	1:E:234:LEU:HD12	2.54	0.43
1:E:65:LEU:HD12	1:E:65:LEU:O	2.19	0.43
1:C:39:ILE:HG23	1:C:54:VAL:HG12	2.01	0.43
1:D:234:LEU:HD21	1:D:240:VAL:HG22	1.99	0.43
1:E:203:ARG:NH1	1:E:266:ASN:HD21	2.17	0.43
1:F:143:LYS:O	1:F:145:PRO:HD3	2.18	0.43
1:F:139:TYR:CE1	1:F:175:ASP:HB3	2.54	0.42
1:E:162:LYS:HG2	1:E:187:GLU:HG3	2.00	0.42
1:D:167:LYS:HG2	1:D:170:ASP:OD2	2.19	0.42
1:E:154:MET:HE2	1:E:163:ARG:NH1	2.33	0.42
1:A:19:TYR:CD1	1:A:23:LYS:HG2	2.55	0.42
1:A:203:ARG:HB3	1:A:264:GLY:HA3	2.01	0.42
1:B:174:MET:HE2	1:B:174:MET:HB2	1.89	0.42
1:A:40:LEU:O	1:A:52:GLY:HA3	2.20	0.42
1:F:279:GLU:O	1:F:280:LEU:HB2	2.19	0.42
1:C:110:MET:HB3	1:C:110:MET:HE2	1.81	0.42
1:C:205:GLU:OE1	1:C:207:TYR:HE1	2.03	0.42
1:F:280:LEU:HD22	1:F:280:LEU:HA	1.65	0.42
1:B:24:LEU:HD23	1:B:24:LEU:HA	1.91	0.42
1:A:2:SER:O	1:A:2:SER:OG	2.37	0.42
1:A:202:ARG:NE	1:B:68:GLU:O	2.53	0.42
1:D:80:LEU:HB3	1:D:108:ILE:HB	2.02	0.41
1:D:218:ARG:HG2	1:D:218:ARG:HH11	1.84	0.41
1:F:202:ARG:H	1:F:202:ARG:HG2	1.75	0.41
1:D:21:THR:HG23	1:F:228:GLU:OE1	2.20	0.41
1:A:227:ASP:HA	1:A:280:LEU:H	1.84	0.41
1:E:106:TYR:CE2	1:E:143:LYS:HB2	2.55	0.41
1:B:180:GLN:HE21	1:B:269:TYR:HE1	1.69	0.41
1:C:227:ASP:O	1:C:280:LEU:HB2	2.21	0.41
1:D:234:LEU:HD21	1:D:240:VAL:CG2	2.51	0.41
1:E:127:LYS:NZ	1:E:237:GLU:OE2	2.47	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLU:CD	1:C:21:THR:HB	2.41	0.41
1:D:154:MET:HE3	1:D:154:MET:HB3	1.90	0.41
1:D:24:LEU:HA	1:D:24:LEU:HD23	1.90	0.41
1:A:70:GLY:HA3	1:B:266:ASN:HD22	1.86	0.41
1:A:236:ASN:ND2	1:A:237:GLU:HG3	2.36	0.41
1:B:182:GLY:HA3	1:B:260:TRP:CE2	2.56	0.41
1:C:220:PHE:CE2	1:C:233:THR:HG23	2.56	0.41
1:E:49:MET:SD	1:E:206:THR:HG21	2.60	0.41
1:E:217:THR:O	1:E:218:ARG:HD2	2.20	0.41
1:F:74:PHE:CD2	1:F:75:LEU:HD13	2.56	0.41
1:F:209:TYR:CE2	1:F:219:VAL:HG11	2.56	0.41
1:C:195:MET:HG2	1:C:196:PRO:HD3	2.02	0.41
1:C:200:HIS:ND1	1:C:203:ARG:O	2.53	0.41
1:B:195:MET:HB3	1:B:196:PRO:HD3	2.03	0.40
1:B:191:SER:OG	1:B:252:GLY:O	2.38	0.40
1:E:236:ASN:ND2	1:E:237:GLU:HG3	2.36	0.40
1:C:236:ASN:ND2	1:C:237:GLU:HG3	2.36	0.40
1:B:103:GLN:O	1:B:168:TYR:OH	2.32	0.40
1:D:91:ILE:O	1:D:98:ASP:N	2.50	0.40
1:C:184:THR:HB	1:C:258:PHE:CE1	2.56	0.40
1:E:24:LEU:HD11	1:E:230:ARG:HB3	2.03	0.40
1:E:148:THR:O	1:E:148:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	277/289 (96%)	263 (95%)	14 (5%)	0	100	100
1	B	277/289 (96%)	265 (96%)	12 (4%)	0	100	100
1	C	277/289 (96%)	263 (95%)	14 (5%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	254/289 (88%)	245 (96%)	9 (4%)	0	100	100
1	E	264/289 (91%)	252 (96%)	12 (4%)	0	100	100
1	F	277/289 (96%)	264 (95%)	13 (5%)	0	100	100
All	All	1626/1734 (94%)	1552 (95%)	74 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	243/253 (96%)	223 (92%)	20 (8%)	11	33
1	B	243/253 (96%)	229 (94%)	14 (6%)	20	50
1	C	243/253 (96%)	225 (93%)	18 (7%)	13	37
1	D	226/253 (89%)	212 (94%)	14 (6%)	18	47
1	E	235/253 (93%)	222 (94%)	13 (6%)	21	52
1	F	243/253 (96%)	230 (95%)	13 (5%)	22	54
All	All	1433/1518 (94%)	1341 (94%)	92 (6%)	17	45

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	THR
1	A	106	TYR
1	A	118	THR
1	A	133	THR
1	A	138	THR
1	A	144	LEU
1	A	163	ARG
1	A	166	TYR
1	A	178	GLN
1	A	179	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	191	SER
1	A	206	THR
1	A	223	LEU
1	A	225	LYS
1	A	233	THR
1	A	270	ASP
1	A	272	MET
1	A	273	ASP
1	A	277	MET
1	A	280	LEU
1	B	106	TYR
1	B	118	THR
1	B	133	THR
1	B	138	THR
1	B	164	THR
1	B	191	SER
1	B	199	THR
1	B	202	ARG
1	B	222	PHE
1	B	233	THR
1	B	251	VAL
1	B	268	THR
1	B	279	GLU
1	B	280	LEU
1	C	22	SER
1	C	54	VAL
1	C	91	ILE
1	C	106	TYR
1	C	133	THR
1	C	150	LEU
1	C	164	THR
1	C	178	GLN
1	C	190	SER
1	C	191	SER
1	C	195	MET
1	C	202	ARG
1	C	204	MET
1	C	206	THR
1	C	235	PHE
1	C	248	HIS
1	C	259	ILE
1	C	272	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	22	SER
1	D	54	VAL
1	D	68	GLU
1	D	72	ASP
1	D	91	ILE
1	D	92	THR
1	D	106	TYR
1	D	118	THR
1	D	191	SER
1	D	200	HIS
1	D	223	LEU
1	D	240	VAL
1	D	241	VAL
1	D	248	HIS
1	E	54	VAL
1	E	67	THR
1	E	91	ILE
1	E	92	THR
1	E	106	TYR
1	E	118	THR
1	E	163	ARG
1	E	240	VAL
1	E	241	VAL
1	E	248	HIS
1	E	251	VAL
1	E	268	THR
1	E	277	MET
1	F	54	VAL
1	F	75	LEU
1	F	106	TYR
1	F	116	VAL
1	F	118	THR
1	F	138	THR
1	F	164	THR
1	F	178	GLN
1	F	191	SER
1	F	202	ARG
1	F	223	LEU
1	F	233	THR
1	F	280	LEU

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

Mol	Chain	Res	Type
1	A	274	GLN
1	D	200	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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EPE	D	301	-	15,15,15	0.73	1 (6%)	18,20,20	2.11	6 (33%)
2	EPE	C	301	-	15,15,15	0.94	1 (6%)	18,20,20	1.99	5 (27%)
2	EPE	E	301	-	15,15,15	0.94	1 (6%)	18,20,20	1.96	5 (27%)
2	EPE	F	301	-	15,15,15	0.73	1 (6%)	18,20,20	1.95	5 (27%)
2	EPE	B	301	-	15,15,15	0.85	1 (6%)	18,20,20	1.84	4 (22%)
2	EPE	A	301	-	15,15,15	0.77	1 (6%)	18,20,20	1.75	4 (22%)

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	EPE	D	301	-	-	4/9/19/19	0/1/1/1
2	EPE	C	301	-	-	5/9/19/19	0/1/1/1
2	EPE	E	301	-	-	3/9/19/19	0/1/1/1
2	EPE	F	301	-	-	3/9/19/19	0/1/1/1
2	EPE	B	301	-	-	7/9/19/19	0/1/1/1
2	EPE	A	301	-	-	6/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	EPE	C10-S	3.27	1.82	1.77
2	E	301	EPE	C10-S	3.24	1.82	1.77
2	B	301	EPE	C10-S	2.89	1.81	1.77
2	D	301	EPE	C10-S	2.49	1.81	1.77
2	A	301	EPE	C10-S	2.47	1.81	1.77
2	F	301	EPE	C10-S	2.35	1.80	1.77

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	EPE	C5-N4-C3	5.41	121.01	108.83
2	F	301	EPE	C5-N4-C3	5.29	120.73	108.83
2	B	301	EPE	C5-N4-C3	4.82	119.67	108.83
2	C	301	EPE	C5-N4-C3	4.03	117.91	108.83
2	C	301	EPE	C7-N4-C5	3.97	121.38	111.23
2	E	301	EPE	C5-N4-C3	3.94	117.71	108.83
2	E	301	EPE	C7-N4-C3	3.78	120.90	111.23
2	A	301	EPE	C5-N4-C3	3.64	117.02	108.83
2	C	301	EPE	C7-N4-C3	3.64	120.54	111.23
2	E	301	EPE	C7-N4-C5	3.57	120.36	111.23
2	A	301	EPE	C7-N4-C3	3.49	120.17	111.23
2	B	301	EPE	C7-N4-C3	3.29	119.66	111.23
2	D	301	EPE	C5-C6-N1	-3.29	103.89	110.64
2	F	301	EPE	C7-N4-C5	3.08	119.12	111.23
2	A	301	EPE	C7-N4-C5	3.02	118.97	111.23
2	F	301	EPE	C7-N4-C3	3.00	118.92	111.23
2	B	301	EPE	C7-N4-C5	2.99	118.89	111.23
2	A	301	EPE	O1S-S-C10	2.93	110.45	106.92
2	D	301	EPE	C7-N4-C5	2.92	118.71	111.23
2	D	301	EPE	C7-N4-C3	2.87	118.58	111.23
2	E	301	EPE	O1S-S-C10	2.71	110.18	106.92
2	C	301	EPE	O3S-S-C10	2.67	110.09	105.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	EPE	O3S-S-C10	2.66	110.06	105.77
2	C	301	EPE	C6-N1-C2	2.64	114.77	108.83
2	E	301	EPE	C6-N1-C2	2.61	114.69	108.83
2	D	301	EPE	C2-C3-N4	2.49	115.76	110.64
2	F	301	EPE	O3S-S-C10	2.41	109.67	105.77
2	B	301	EPE	C3-C2-N1	-2.12	106.30	110.64
2	F	301	EPE	C9-N1-C6	-2.09	105.89	111.23

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	EPE	N4-C7-C8-O8
2	B	301	EPE	S-C10-C9-N1
2	B	301	EPE	C9-C10-S-O2S
2	B	301	EPE	C9-C10-S-O3S
2	C	301	EPE	S-C10-C9-N1
2	D	301	EPE	C8-C7-N4-C5
2	D	301	EPE	C9-C10-S-O1S
2	E	301	EPE	S-C10-C9-N1
2	F	301	EPE	C9-C10-S-O3S
2	A	301	EPE	C9-C10-S-O3S
2	C	301	EPE	C8-C7-N4-C3
2	A	301	EPE	C10-C9-N1-C2
2	B	301	EPE	C10-C9-N1-C6
2	C	301	EPE	C10-C9-N1-C6
2	D	301	EPE	C10-C9-N1-C2
2	D	301	EPE	C10-C9-N1-C6
2	E	301	EPE	C8-C7-N4-C5
2	A	301	EPE	C9-C10-S-O1S
2	A	301	EPE	C9-C10-S-O2S
2	B	301	EPE	C9-C10-S-O1S
2	F	301	EPE	C9-C10-S-O1S
2	F	301	EPE	C9-C10-S-O2S
2	A	301	EPE	C8-C7-N4-C5
2	B	301	EPE	C10-C9-N1-C2
2	C	301	EPE	C10-C9-N1-C2
2	E	301	EPE	C10-C9-N1-C6
2	C	301	EPE	C8-C7-N4-C5
2	A	301	EPE	C10-C9-N1-C6

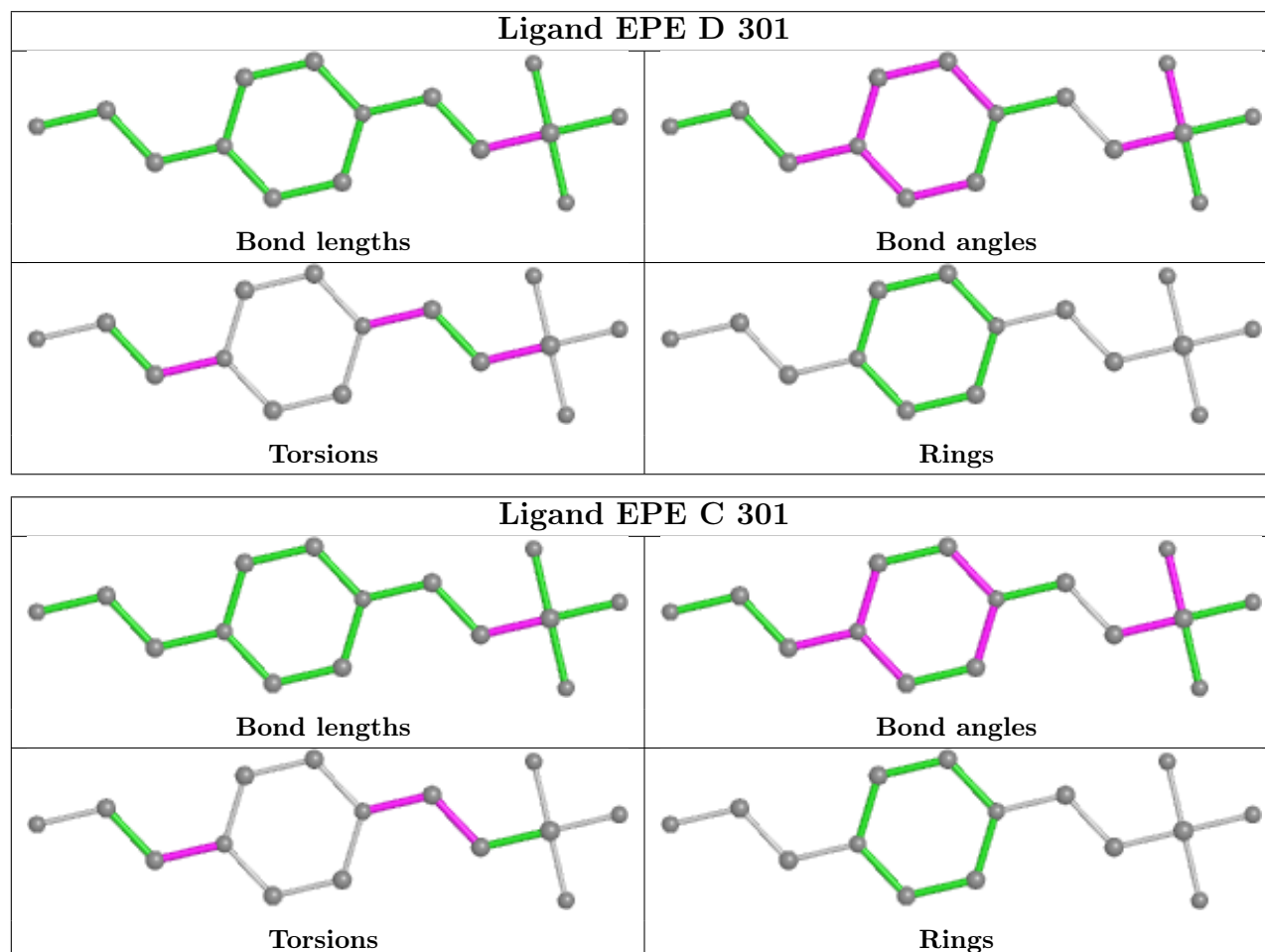
There are no ring outliers.

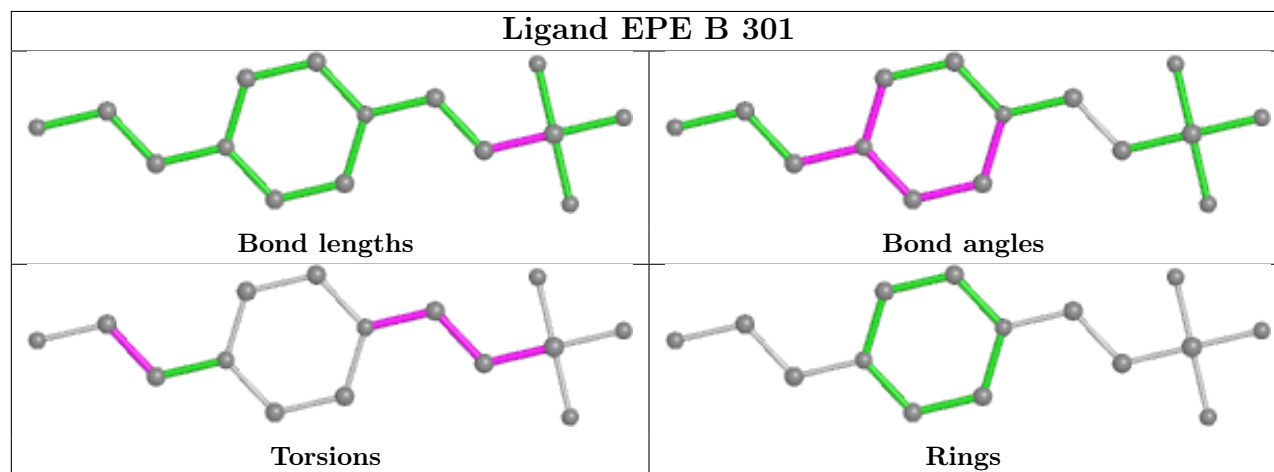
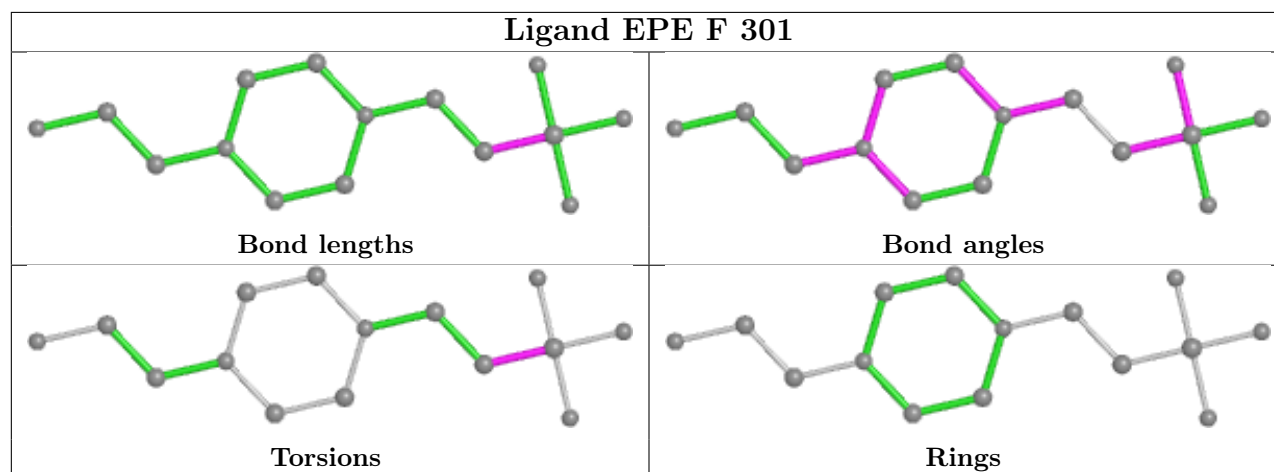
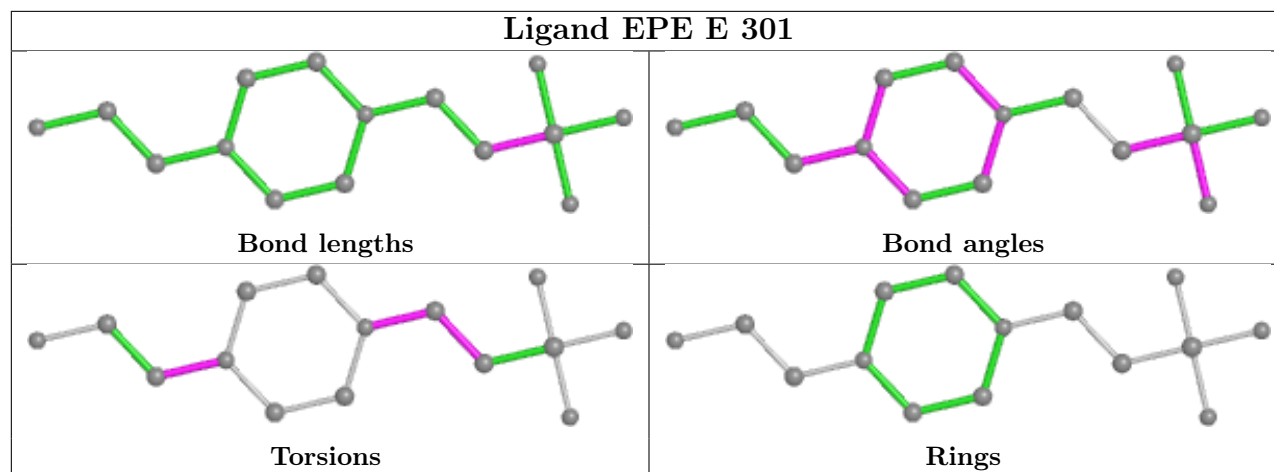


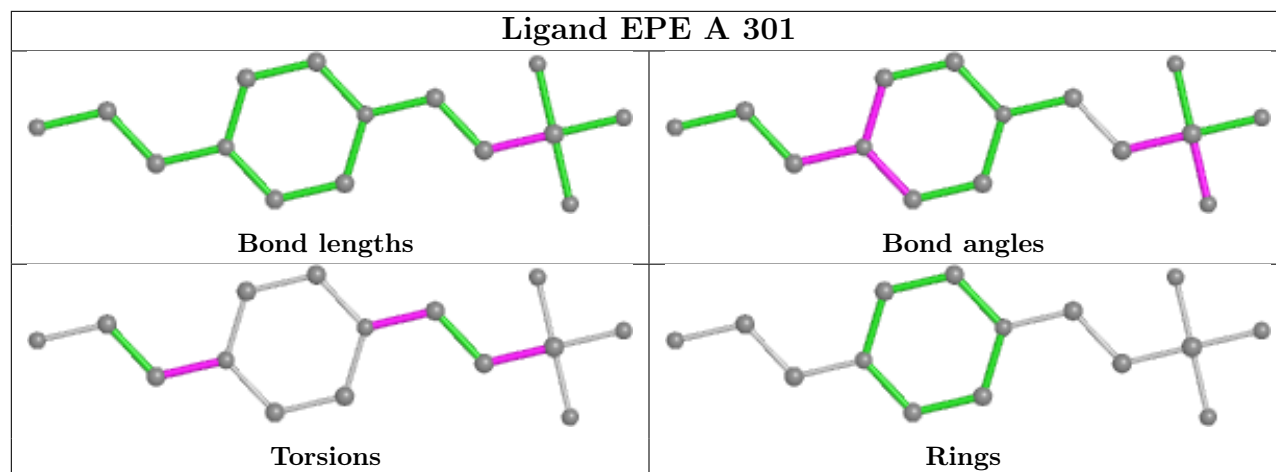
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	EPE	1	0
2	F	301	EPE	3	0
2	B	301	EPE	1	0
2	A	301	EPE	4	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	279/289 (96%)	-0.00	3 (1%) 80 75	56, 82, 131, 155	0
1	B	279/289 (96%)	0.06	3 (1%) 80 75	51, 79, 122, 144	0
1	C	279/289 (96%)	0.15	11 (3%) 39 29	61, 96, 139, 164	0
1	D	260/289 (89%)	-0.23	0 100 100	53, 81, 117, 156	0
1	E	270/289 (93%)	0.29	9 (3%) 46 36	59, 88, 141, 182	0
1	F	279/289 (96%)	0.02	4 (1%) 75 70	51, 88, 141, 181	0
All	All	1646/1734 (94%)	0.05	30 (1%) 68 61	51, 85, 131, 182	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	LYS	4.4
1	E	275	VAL	3.7
1	F	99	ALA	3.0
1	B	124	HIS	2.9
1	C	150	LEU	2.9
1	E	56	PRO	2.9
1	E	268	THR	2.7
1	F	96	ARG	2.7
1	E	128	PHE	2.7
1	C	269	TYR	2.6
1	E	85	ILE	2.6
1	C	106	TYR	2.6
1	C	105	GLY	2.5
1	B	123	ASP	2.5
1	C	144	LEU	2.5
1	C	168	TYR	2.5
1	E	195	MET	2.4
1	A	155	GLY	2.4
1	C	149	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	54	VAL	2.3
1	F	87	GLY	2.3
1	C	267	GLN	2.2
1	A	280	LEU	2.1
1	F	95	GLY	2.1
1	B	121	ASP	2.1
1	E	39	ILE	2.1
1	C	181	MET	2.1
1	C	82	ILE	2.0
1	C	166	TYR	2.0
1	E	117	PHE	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](#)

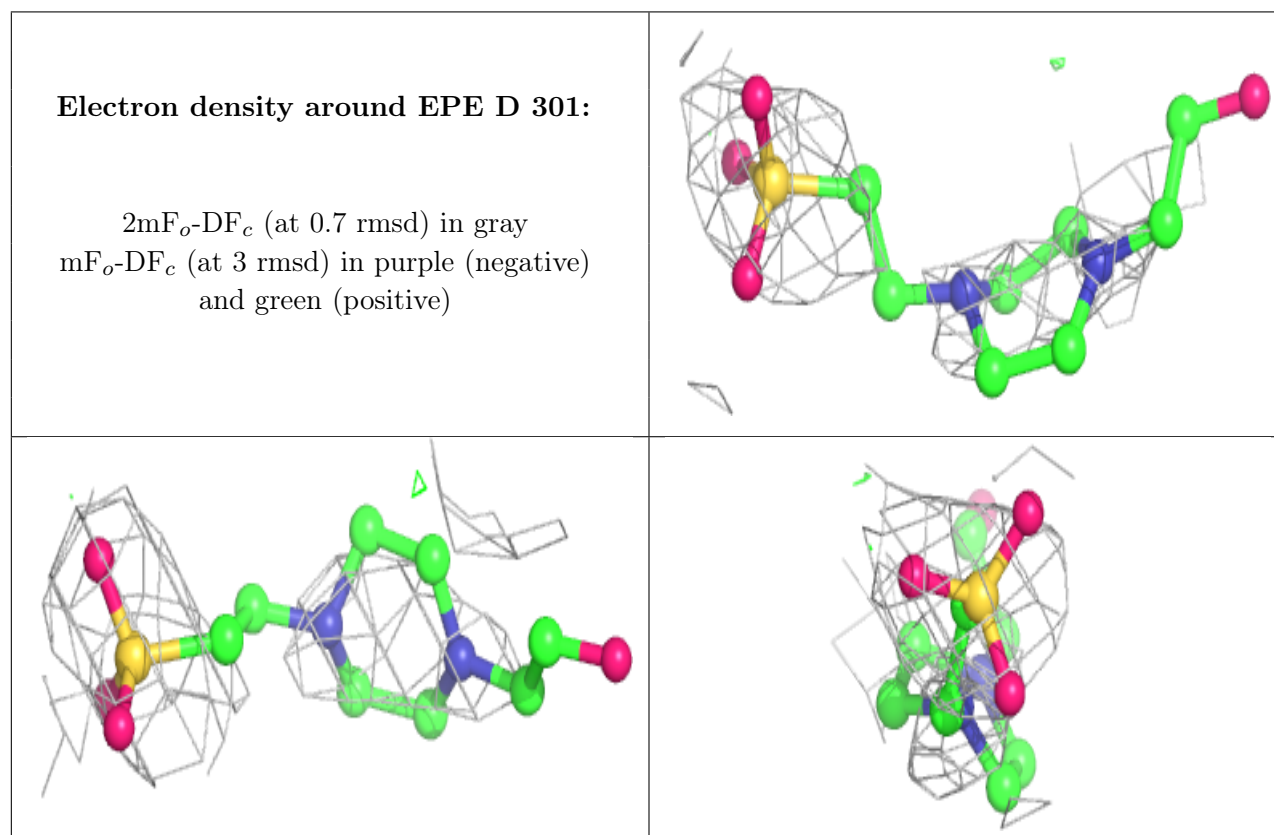
There are no monosaccharides in this entry.

## 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.

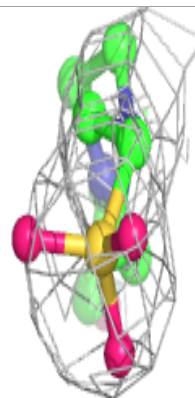
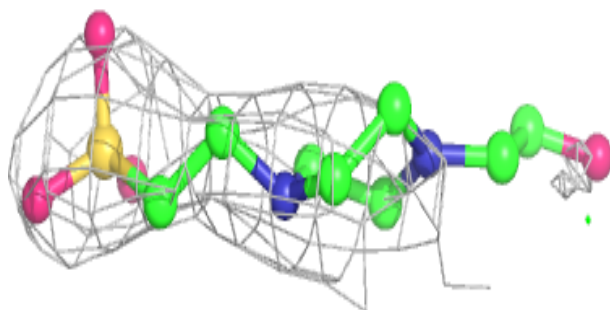
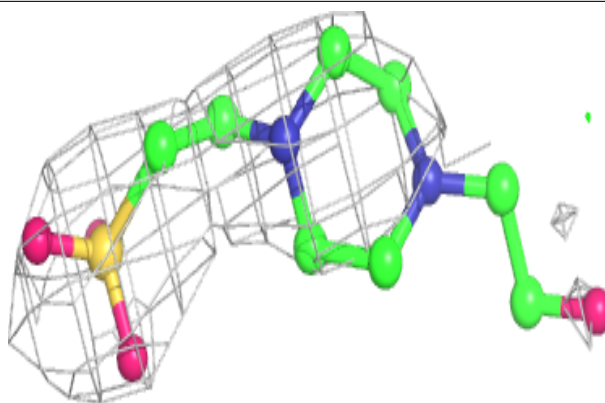
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	EPE	D	301	15/15	0.73	0.44	142,164,180,183	0
3	ZN	E	302	1/1	0.84	0.10	130,130,130,130	0
2	EPE	C	301	15/15	0.85	0.40	126,133,151,151	0
2	EPE	B	301	15/15	0.90	0.23	111,122,129,130	0
3	ZN	D	302	1/1	0.91	0.06	126,126,126,126	0
2	EPE	E	301	15/15	0.91	0.20	123,130,146,149	0
2	EPE	A	301	15/15	0.92	0.28	102,121,131,132	0
2	EPE	F	301	15/15	0.92	0.17	99,111,138,142	0
3	ZN	B	302	1/1	0.96	0.17	128,128,128,128	0
3	ZN	A	302	1/1	0.97	0.06	102,102,102,102	0
3	ZN	C	302	1/1	0.97	0.06	112,112,112,112	0
3	ZN	F	302	1/1	0.98	0.09	118,118,118,118	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.

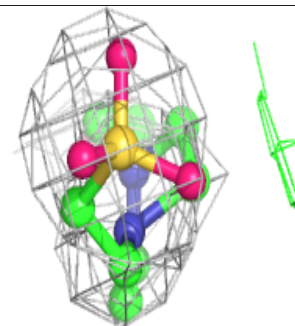
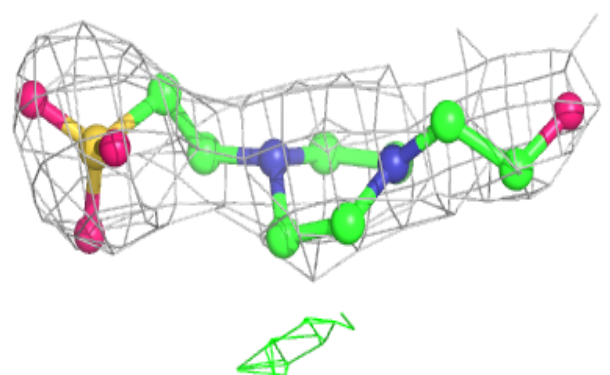
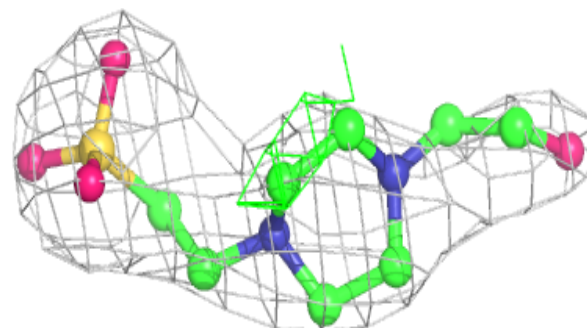


**Electron density around EPE C 301:**

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

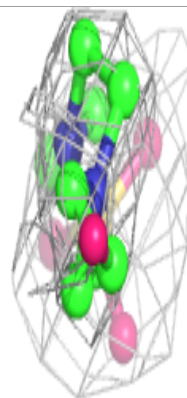
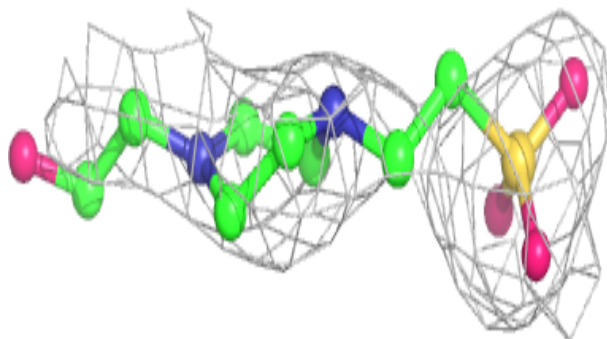
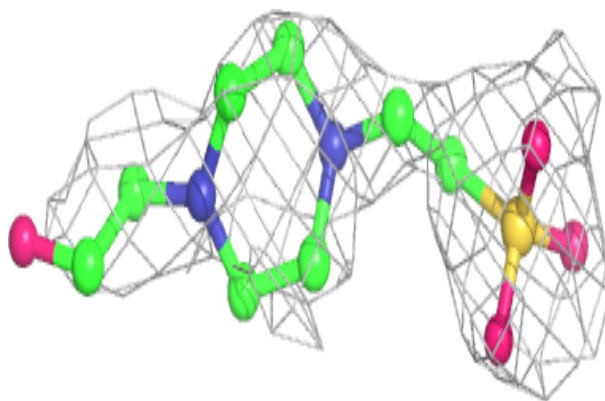
**Electron density around EPE B 301:**

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

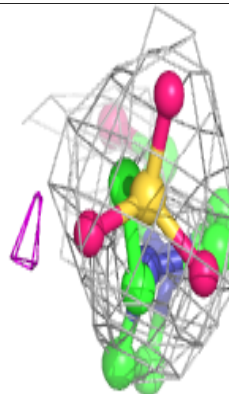
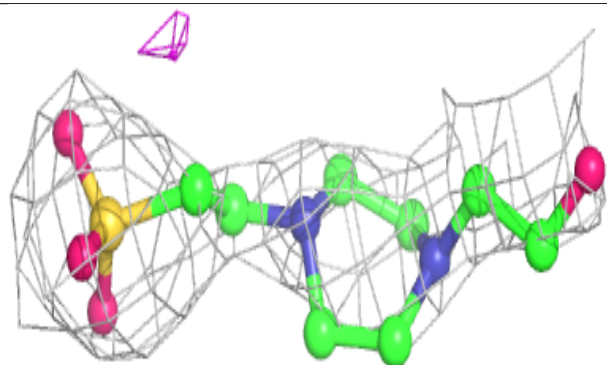
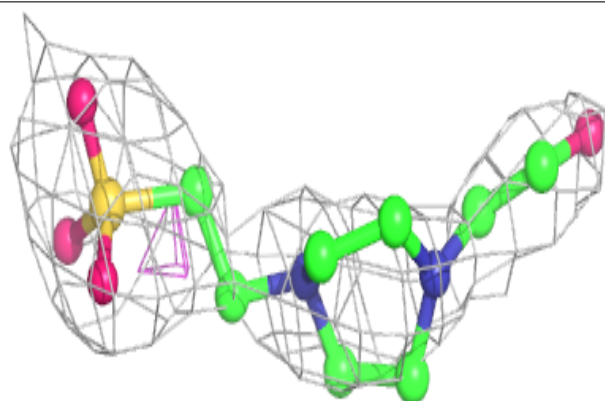


**Electron density around EPE E 301:**

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

**Electron density around EPE A 301:**

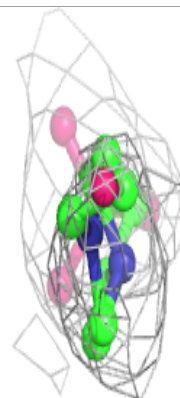
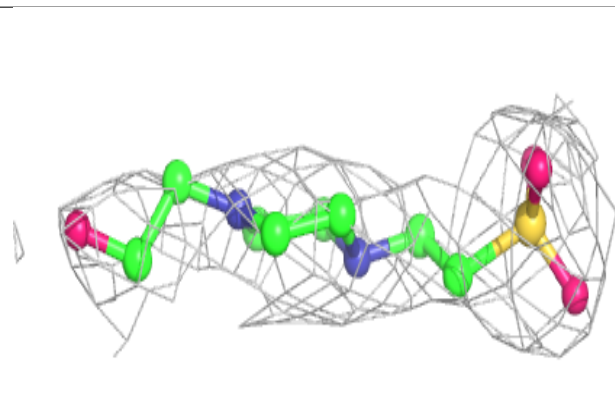
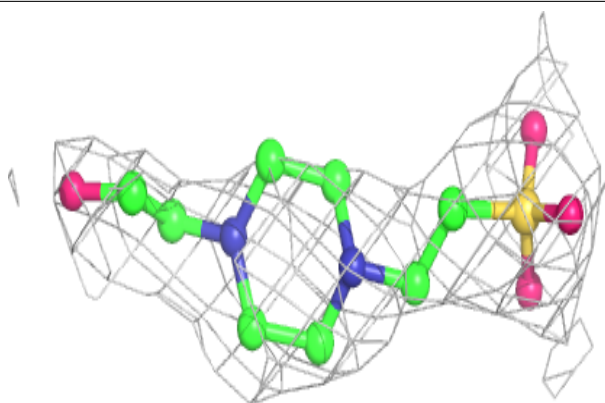
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around EPE F 301:**

$2mF_o - DF_c$  (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.