



# Full wwPDB X-ray Structure Validation Report i

Aug 7, 2023 – 10:09 PM JST

PDB ID : 7YRS  
Title : Crystal structure of Lactobacillus rhamnosus 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase KduI complexed with MOPS  
Authors : Yamamoto, Y.; Oiki, S.; Takase, R.; Mikami, B.; Hashimoto, W.  
Deposited on : 2022-08-10  
Resolution : 2.80 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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) i) 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 : 2.35  
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) : 2.35

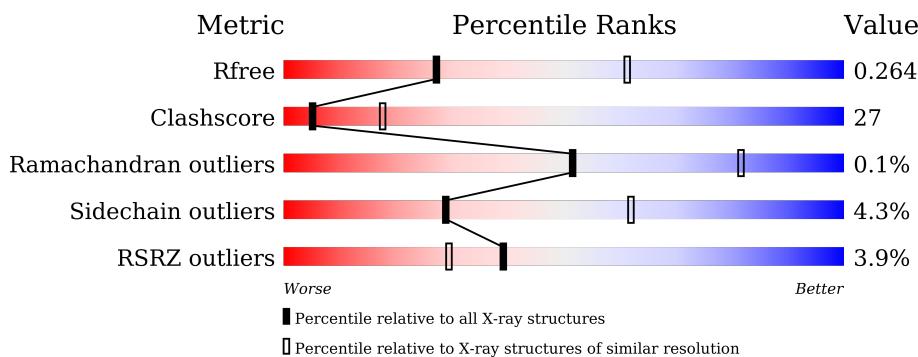
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 >=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 <=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.



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13304 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 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total 2243	C 1423	N 378	O 424	S 18	0	0	0
1	B	276	Total 2219	C 1408	N 374	O 420	S 17	0	0	0
1	C	279	Total 2243	C 1423	N 378	O 424	S 18	0	0	0
1	D	261	Total 2100	C 1337	N 355	O 392	S 16	0	0	0
1	E	276	Total 2222	C 1409	N 375	O 421	S 17	0	0	0
1	F	276	Total 2219	C 1411	N 374	O 416	S 18	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	LEU	-	expression tag	UNP C2JUP1
A	283	GLU	-	expression tag	UNP C2JUP1
A	284	HIS	-	expression tag	UNP C2JUP1
A	285	HIS	-	expression tag	UNP C2JUP1
A	286	HIS	-	expression tag	UNP C2JUP1
A	287	HIS	-	expression tag	UNP C2JUP1
A	288	HIS	-	expression tag	UNP C2JUP1
A	289	HIS	-	expression tag	UNP C2JUP1
B	282	LEU	-	expression tag	UNP C2JUP1
B	283	GLU	-	expression tag	UNP C2JUP1
B	284	HIS	-	expression tag	UNP C2JUP1
B	285	HIS	-	expression tag	UNP C2JUP1
B	286	HIS	-	expression tag	UNP C2JUP1
B	287	HIS	-	expression tag	UNP C2JUP1
B	288	HIS	-	expression tag	UNP C2JUP1
B	289	HIS	-	expression tag	UNP C2JUP1
C	282	LEU	-	expression tag	UNP C2JUP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	283	GLU	-	expression tag	UNP C2JUP1
C	284	HIS	-	expression tag	UNP C2JUP1
C	285	HIS	-	expression tag	UNP C2JUP1
C	286	HIS	-	expression tag	UNP C2JUP1
C	287	HIS	-	expression tag	UNP C2JUP1
C	288	HIS	-	expression tag	UNP C2JUP1
C	289	HIS	-	expression tag	UNP C2JUP1
D	282	LEU	-	expression tag	UNP C2JUP1
D	283	GLU	-	expression tag	UNP C2JUP1
D	284	HIS	-	expression tag	UNP C2JUP1
D	285	HIS	-	expression tag	UNP C2JUP1
D	286	HIS	-	expression tag	UNP C2JUP1
D	287	HIS	-	expression tag	UNP C2JUP1
D	288	HIS	-	expression tag	UNP C2JUP1
D	289	HIS	-	expression tag	UNP C2JUP1
E	282	LEU	-	expression tag	UNP C2JUP1
E	283	GLU	-	expression tag	UNP C2JUP1
E	284	HIS	-	expression tag	UNP C2JUP1
E	285	HIS	-	expression tag	UNP C2JUP1
E	286	HIS	-	expression tag	UNP C2JUP1
E	287	HIS	-	expression tag	UNP C2JUP1
E	288	HIS	-	expression tag	UNP C2JUP1
E	289	HIS	-	expression tag	UNP C2JUP1
F	282	LEU	-	expression tag	UNP C2JUP1
F	283	GLU	-	expression tag	UNP C2JUP1
F	284	HIS	-	expression tag	UNP C2JUP1
F	285	HIS	-	expression tag	UNP C2JUP1
F	286	HIS	-	expression tag	UNP C2JUP1
F	287	HIS	-	expression tag	UNP C2JUP1
F	288	HIS	-	expression tag	UNP C2JUP1
F	289	HIS	-	expression tag	UNP C2JUP1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

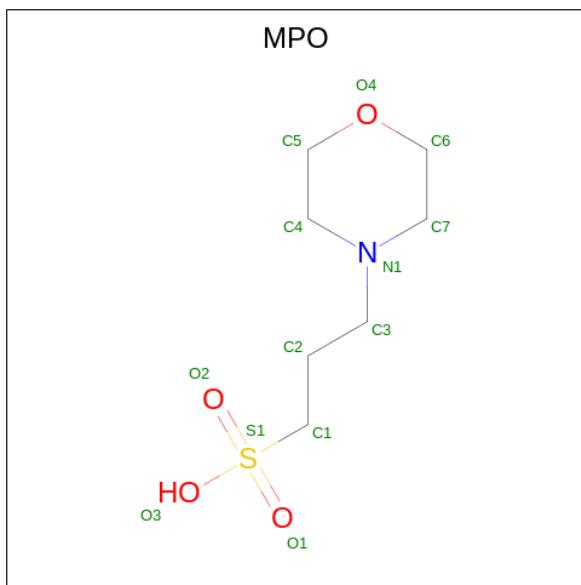
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).

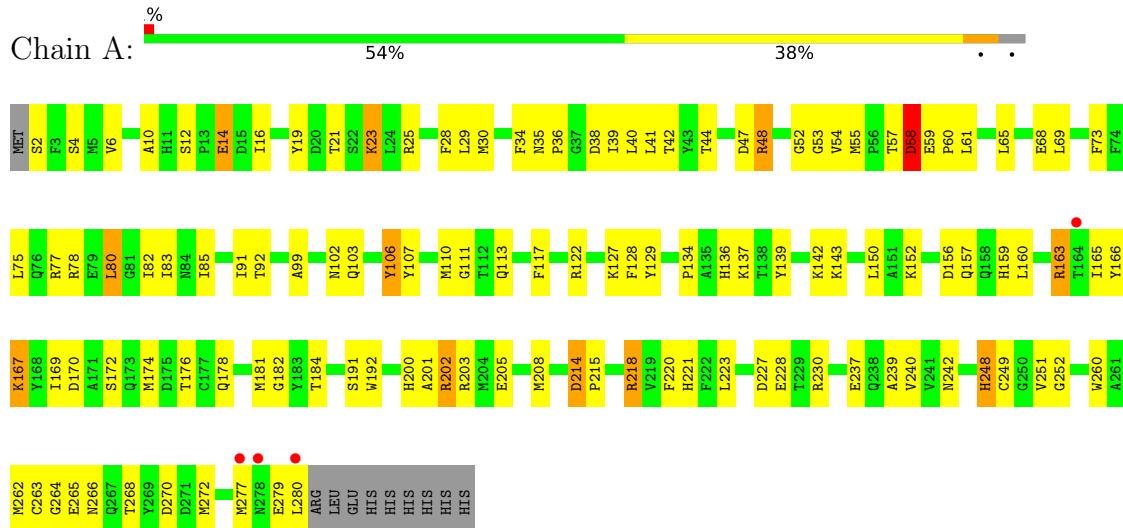


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 13 7 1 4 1	0	0
3	B	1	Total C N O S 13 7 1 4 1	0	0
3	E	1	Total C N O S 13 7 1 4 1	0	0
3	F	1	Total C N O S 13 7 1 4 1	0	0

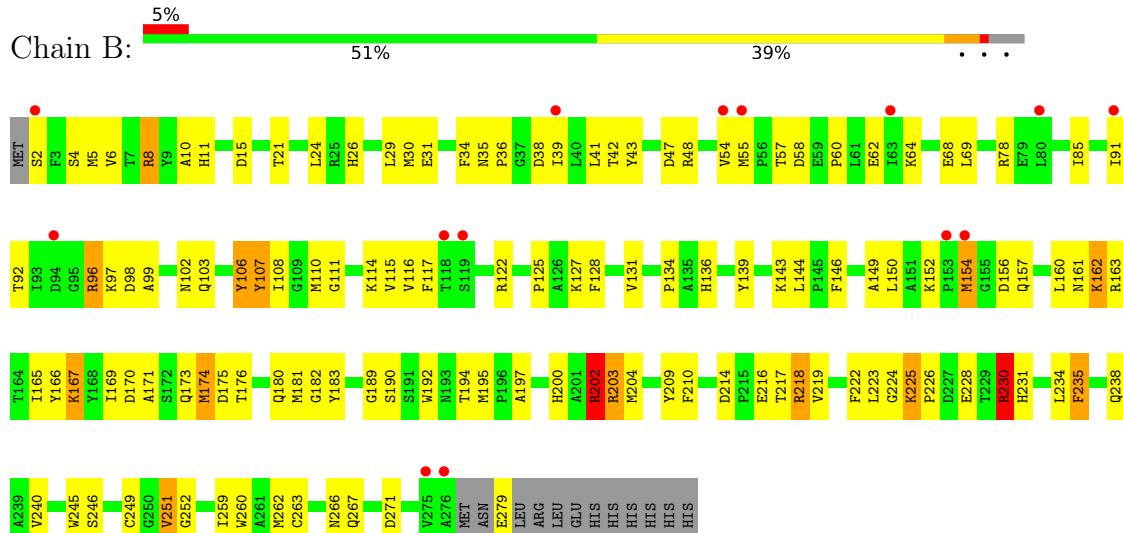
### 3 Residue-property plots [\(i\)](#)

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: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase

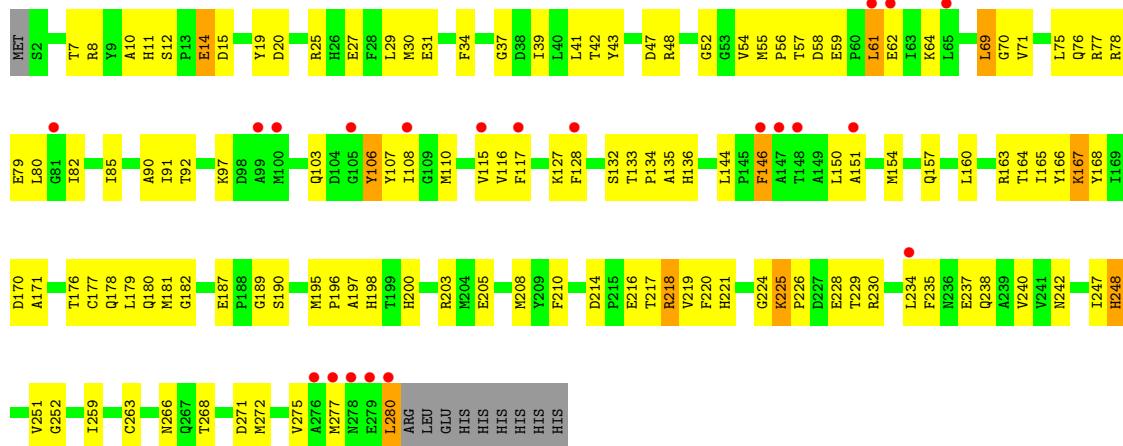


- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



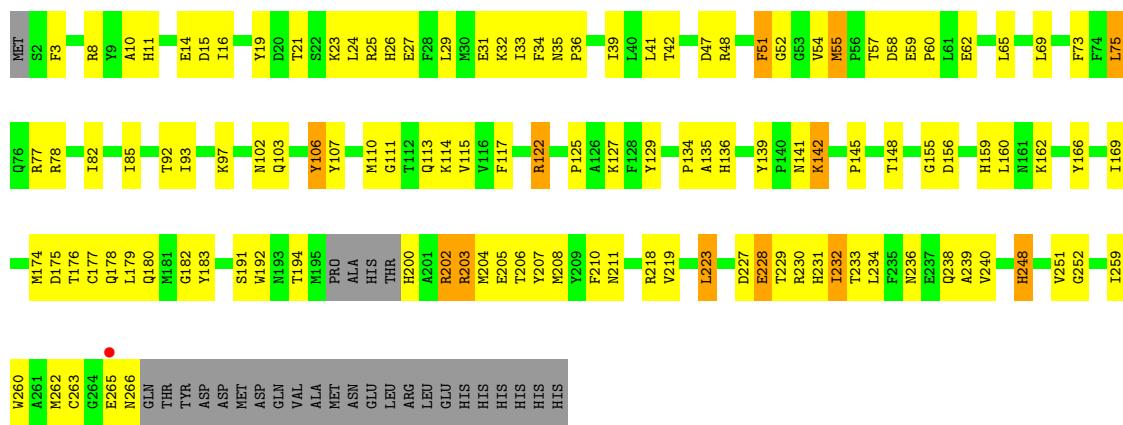
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase





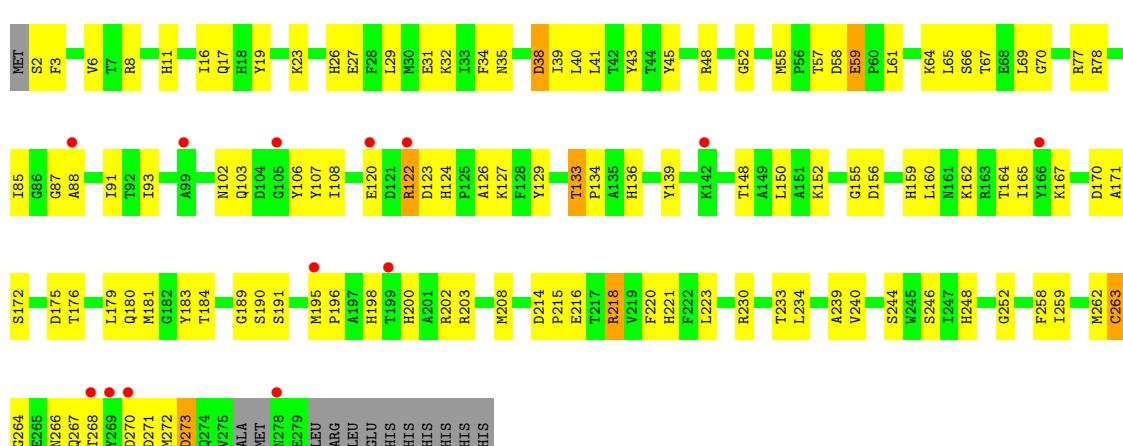
- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase

Chain D:

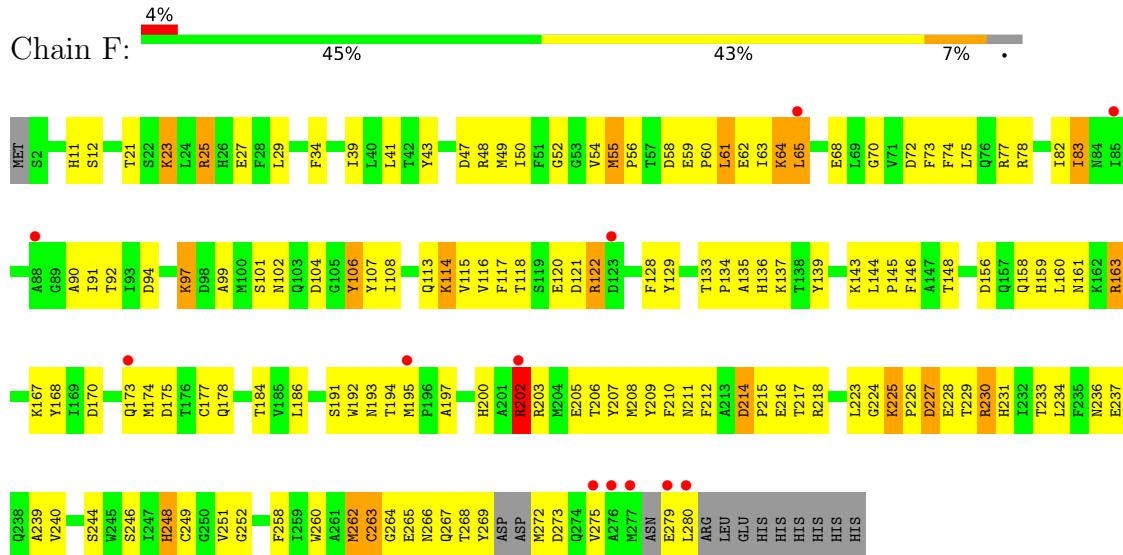


- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase

Class E



- Molecule 1: 4-deoxy-L-threo-5-hexosulose-uronate ketol-isomerase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.40 Å    187.40 Å    108.93 Å 90.00°    112.49°    90.00°	Depositor
Resolution (Å)	49.55 – 2.80 49.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.55-2.80) 99.1 (49.55-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.75 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
$R$ , $R_{free}$	0.189 , 0.265 0.190 , 0.264	Depositor DCC
$R_{free}$ test set	2034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: MPO, ZN

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	0.57	1/2303 (0.0%)	0.93	12/3121 (0.4%)
1	B	0.71	6/2278 (0.3%)	0.99	10/3086 (0.3%)
1	C	0.65	4/2303 (0.2%)	0.96	10/3121 (0.3%)
1	D	0.63	3/2156 (0.1%)	0.98	10/2918 (0.3%)
1	E	0.53	2/2281 (0.1%)	0.89	5/3090 (0.2%)
1	F	0.74	10/2277 (0.4%)	1.02	15/3082 (0.5%)
All	All	0.64	26/13598 (0.2%)	0.96	62/18418 (0.3%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	202	ARG	CG-CD	-10.10	1.26	1.51
1	D	202	ARG	CZ-NH1	-8.82	1.21	1.33
1	D	202	ARG	NE-CZ	-8.11	1.22	1.33
1	B	202	ARG	CZ-NH1	-8.09	1.22	1.33
1	F	202	ARG	NE-CZ	-7.86	1.22	1.33
1	F	216	GLU	CD-OE1	-7.42	1.17	1.25
1	C	14	GLU	CD-OE1	-7.39	1.17	1.25
1	F	216	GLU	CG-CD	-6.79	1.41	1.51
1	B	251	VAL	CB-CG1	-6.73	1.38	1.52
1	A	58	ASP	C-N	6.65	1.49	1.34
1	F	23	LYS	CD-CE	-6.60	1.34	1.51
1	C	235	PHE	CE2-CZ	-6.44	1.25	1.37
1	B	202	ARG	NE-CZ	-6.37	1.24	1.33
1	B	203	ARG	CZ-NH1	-6.16	1.25	1.33
1	F	202	ARG	CZ-NH1	-6.15	1.25	1.33
1	C	14	GLU	CD-OE2	-6.12	1.19	1.25
1	E	59	GLU	CD-OE1	-6.08	1.19	1.25
1	E	59	GLU	CB-CG	5.78	1.63	1.52
1	F	23	LYS	CE-NZ	-5.77	1.34	1.49
1	F	202	ARG	CZ-NH2	-5.67	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202	ARG	CZ-NH2	-5.66	1.25	1.33
1	B	203	ARG	CZ-NH2	-5.56	1.25	1.33
1	B	203	ARG	NE-CZ	-5.37	1.26	1.33
1	C	235	PHE	CE1-CZ	-5.34	1.27	1.37
1	F	64	LYS	CE-NZ	-5.32	1.35	1.49
1	F	216	GLU	CB-CG	-5.17	1.42	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ARG	CG-CD-NE	-14.40	81.57	111.80
1	F	202	ARG	NE-CZ-NH1	-13.89	113.35	120.30
1	E	122	ARG	CB-CG-CD	-13.46	76.62	111.60
1	B	218	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	F	144	LEU	CA-CB-CG	9.33	136.75	115.30
1	A	48	ARG	NE-CZ-NH1	-8.93	115.84	120.30
1	C	69	LEU	CA-CB-CG	8.80	135.53	115.30
1	D	75	LEU	CB-CG-CD2	-8.74	96.15	111.00
1	F	122	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	218	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	D	232	ILE	CG1-CB-CG2	-8.27	93.21	111.40
1	C	218	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	E	122	ARG	CA-CB-CG	8.16	131.35	113.40
1	F	65	LEU	CB-CG-CD2	8.06	124.71	111.00
1	D	114	LYS	CA-CB-CG	7.66	130.25	113.40
1	D	114	LYS	CB-CG-CD	-7.63	91.77	111.60
1	F	230	ARG	NE-CZ-NH1	-7.53	116.53	120.30
1	A	167	LYS	CD-CE-NZ	-7.49	94.48	111.70
1	B	64	LYS	CA-CB-CG	7.42	129.73	113.40
1	D	75	LEU	CA-CB-CG	-7.12	98.93	115.30
1	D	122	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	D	75	LEU	CB-CG-CD1	7.08	123.03	111.00
1	B	202	ARG	CG-CD-NE	7.05	126.61	111.80
1	B	235	PHE	CB-CG-CD1	7.00	125.70	120.80
1	C	167	LYS	CA-CB-CG	6.89	128.56	113.40
1	F	202	ARG	CG-CD-NE	-6.80	97.52	111.80
1	B	202	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	F	225	LYS	CB-CG-CD	-6.67	94.26	111.60
1	A	218	ARG	CG-CD-NE	-6.57	98.01	111.80
1	D	55	MET	CA-CB-CG	6.52	124.38	113.30
1	A	214	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	154	MET	N-CA-CB	-6.22	99.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASP	C-N-CA	6.14	137.05	121.70
1	A	80	LEU	CA-CB-CG	6.06	129.25	115.30
1	C	25	ARG	CG-CD-NE	6.06	124.52	111.80
1	C	61	LEU	CB-CA-C	6.02	121.65	110.20
1	F	120	GLU	CA-CB-CG	6.02	126.64	113.40
1	C	235	PHE	CB-CG-CD2	5.90	124.93	120.80
1	E	59	GLU	N-CA-CB	-5.77	100.21	110.60
1	A	167	LYS	CB-CG-CD	-5.77	96.60	111.60
1	C	77	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	F	163	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	58	ASP	CB-CG-OD1	5.67	123.41	118.30
1	D	203	ARG	CA-CB-CG	5.67	125.87	113.40
1	E	218	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	A	218	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	202	ARG	CB-CA-C	-5.41	99.57	110.40
1	F	64	LYS	CA-CB-CG	5.27	124.99	113.40
1	F	25	ARG	CB-CG-CD	5.24	125.23	111.60
1	B	230	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	A	48	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	F	122	ARG	CG-CD-NE	-5.21	100.86	111.80
1	C	280	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	154	MET	CG-SD-CE	-5.16	91.94	100.20
1	B	162	LYS	CA-CB-CG	5.14	124.72	113.40
1	F	227	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	25	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	122	ARG	CD-NE-CZ	5.07	130.70	123.60
1	E	38	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	14	GLU	N-CA-CB	-5.05	101.52	110.60
1	F	262	MET	CB-CG-SD	-5.02	97.33	112.40
1	B	152	LYS	N-CA-CB	5.00	119.60	110.60

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	113	0
1	B	2219	0	2117	154	0
1	C	2243	0	2144	129	0
1	D	2100	0	2018	119	0
1	E	2222	0	2118	112	0
1	F	2219	0	2128	148	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	13	0	14	1	0
3	B	13	0	14	2	0
3	E	13	0	15	0	0
3	F	13	0	15	4	0
All	All	13304	0	12727	698	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 27.

All (698) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TYR:CG	1:A:23:LYS:NZ	2.00	1.28
1:B:154:MET:HE1	1:B:163:ARG:NH1	1.51	1.24
1:D:75:LEU:HD12	1:D:78:ARG:HB2	1.31	1.08
1:A:19:TYR:CD2	1:A:23:LYS:NZ	2.21	1.07
1:B:154:MET:CE	1:B:163:ARG:CZ	2.34	1.06
1:F:92:THR:HG22	1:F:97:LYS:HG3	1.38	1.06
1:E:48:ARG:NH1	1:F:47:ASP:OD1	1.91	1.03
1:A:279:GLU:H	1:E:218:ARG:HH12	1.07	0.99
1:B:154:MET:CE	1:B:163:ARG:NH1	2.27	0.98
1:A:142:LYS:NZ	1:A:174:MET:HB3	1.77	0.98
1:B:154:MET:HE1	1:B:163:ARG:CZ	1.93	0.98
1:F:228:GLU:HG3	1:F:230:ARG:HH12	1.29	0.97
1:B:216:GLU:HB3	1:C:277:MET:HG3	1.44	0.97
1:C:78:ARG:NH1	1:D:265:GLU:OE2	2.01	0.94
1:B:154:MET:HE3	1:B:163:ARG:NE	1.83	0.93
1:D:75:LEU:CD1	1:D:78:ARG:HB2	1.98	0.93
1:B:154:MET:HE1	1:B:163:ARG:HH11	1.20	0.93
1:B:39:ILE:HD13	1:B:54:VAL:HG12	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ALA:O	1:F:143:LYS:NZ	2.04	0.90
1:B:85:ILE:HD11	1:B:210:PHE:CG	2.07	0.89
1:D:203:ARG:HB2	1:D:263:CYS:O	1.71	0.88
1:F:65:LEU:HD22	1:F:68:GLU:OE1	1.72	0.88
1:A:48:ARG:NH1	1:B:47:ASP:OD1	2.07	0.87
1:D:55:MET:HE3	1:D:127:LYS:HG2	1.54	0.87
1:B:154:MET:CE	1:B:163:ARG:NE	2.37	0.87
1:A:69:LEU:HA	1:B:202:ARG:NE	1.91	0.86
1:A:142:LYS:HZ3	1:A:174:MET:HB3	1.41	0.84
1:F:225:LYS:NZ	1:F:225:LYS:HB3	1.91	0.84
1:B:131:VAL:HB	1:B:181:MET:HE2	1.60	0.83
1:D:16:ILE:O	1:D:230:ARG:NH2	2.13	0.82
1:C:92:THR:OG1	1:C:116:VAL:HG12	1.81	0.81
1:B:99:ALA:O	1:B:143:LYS:NZ	2.14	0.80
1:F:58:ASP:HB2	1:F:122:ARG:NH1	1.96	0.80
1:F:163:ARG:NH1	3:F:302:MPO:O3	2.15	0.79
1:C:226:PRO:HB3	1:C:275:VAL:HG21	1.64	0.79
1:A:279:GLU:H	1:E:218:ARG:NH1	1.80	0.78
1:A:279:GLU:N	1:E:218:ARG:HH12	1.81	0.78
1:E:85:ILE:HD11	1:E:259:ILE:HD11	1.65	0.78
1:C:136:HIS:H	1:D:136:HIS:HD2	1.32	0.77
1:C:221:HIS:HE1	1:C:242:ASN:HD21	1.32	0.77
1:A:48:ARG:HH12	1:B:47:ASP:CG	1.86	0.77
1:A:200:HIS:NE2	1:A:205:GLU:OE2	2.14	0.77
1:A:160:LEU:HD23	1:E:160:LEU:HD23	1.67	0.77
1:D:32:LYS:HD3	1:D:33:ILE:H	1.47	0.77
1:E:48:ARG:O	1:E:78:ARG:NH2	2.18	0.77
1:E:200:HIS:HB3	1:E:272:MET:HE1	1.64	0.77
1:F:167:LYS:HD2	1:F:173:GLN:HB2	1.65	0.77
1:E:267:GLN:HE21	1:F:77:ARG:HH22	1.30	0.77
1:D:203:ARG:HH11	1:D:263:CYS:HA	1.50	0.77
1:E:203:ARG:NH2	1:E:268:THR:O	2.18	0.77
1:C:266:ASN:ND2	1:C:268:THR:H	1.83	0.76
1:C:78:ARG:HD2	1:C:132:SER:OG	1.85	0.76
1:A:169:ILE:HD12	1:A:181:MET:HG3	1.68	0.76
1:F:92:THR:HG22	1:F:97:LYS:CG	2.16	0.76
1:A:19:TYR:CB	1:A:23:LYS:NZ	2.48	0.76
1:D:191:SER:OG	1:D:252:GLY:N	2.18	0.76
1:D:233:THR:HG23	1:F:280:LEU:HD22	1.68	0.75
1:C:266:ASN:HD21	1:C:268:THR:HG23	1.51	0.75
1:A:19:TYR:HB3	1:A:23:LYS:HZ1	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:HZ1	1:A:174:MET:HB3	1.50	0.75
1:B:214:ASP:HB3	1:B:217:THR:OG1	1.87	0.75
1:B:114:LYS:HE2	1:B:116:VAL:HB	1.68	0.75
1:D:75:LEU:HD12	1:D:78:ARG:CB	2.13	0.74
1:E:8:ARG:NH1	1:E:26:HIS:O	2.19	0.74
1:E:200:HIS:HB2	1:E:202:ARG:NH2	2.02	0.74
1:B:225:LYS:H	1:B:225:LYS:HD3	1.51	0.74
1:E:32:LYS:HE3	1:E:35:ASN:HB2	1.69	0.73
1:C:136:HIS:H	1:D:136:HIS:CD2	2.06	0.73
1:B:160:LEU:HD23	1:C:160:LEU:HD23	1.71	0.72
1:D:32:LYS:HD3	1:D:33:ILE:N	2.04	0.72
1:D:174:MET:HG2	1:D:175:ASP:H	1.55	0.72
1:D:160:LEU:HD23	1:F:160:LEU:HD23	1.71	0.72
1:E:78:ARG:NH1	1:F:265:GLU:OE1	2.22	0.72
1:D:39:ILE:HG12	1:D:54:VAL:HG13	1.72	0.71
1:D:59:GLU:HG3	1:D:60:PRO:HD2	1.73	0.71
1:F:210:PHE:HD2	1:F:211:ASN:HD22	1.38	0.71
1:E:202:ARG:HH21	1:E:203:ARG:NH1	1.87	0.71
1:F:228:GLU:CG	1:F:230:ARG:HH12	2.03	0.71
1:E:69:LEU:C	1:F:202:ARG:HH12	1.94	0.71
1:E:266:ASN:ND2	1:F:70:GLY:O	2.24	0.71
1:B:225:LYS:HE2	1:B:228:GLU:HB3	1.72	0.70
1:E:195:MET:HB3	1:E:196:PRO:HD3	1.73	0.70
1:B:54:VAL:HG22	1:B:128:PHE:HB2	1.74	0.70
1:E:129:TYR:CE1	1:E:208:MET:HG3	2.27	0.69
1:F:167:LYS:HG3	1:F:170:ASP:HB3	1.74	0.69
1:F:203:ARG:HB2	1:F:263:CYS:O	1.92	0.69
1:D:19:TYR:O	1:D:230:ARG:NH1	2.19	0.69
1:D:19:TYR:CD1	1:D:23:LYS:HG2	2.27	0.69
1:E:34:PHE:HZ	1:E:129:TYR:HB2	1.57	0.69
1:B:21:THR:HG23	1:C:230:ARG:HH12	1.57	0.69
1:D:16:ILE:HA	1:D:19:TYR:CD2	2.26	0.69
1:F:56:PRO:HG2	1:F:128:PHE:HE2	1.56	0.69
1:F:225:LYS:HB3	1:F:225:LYS:HZ2	1.54	0.69
1:F:200:HIS:ND1	1:F:203:ARG:O	2.23	0.69
1:D:203:ARG:NH2	1:D:266:ASN:O	2.20	0.68
1:A:191:SER:OG	1:A:252:GLY:N	2.26	0.68
1:A:200:HIS:ND1	1:A:203:ARG:O	2.26	0.68
1:F:191:SER:HB2	1:F:252:GLY:H	1.58	0.68
1:B:161:ASN:HB2	1:B:163:ARG:NH2	2.08	0.68
1:B:154:MET:HE3	1:B:163:ARG:CZ	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:VAL:HA	1:C:252:GLY:HA2	1.74	0.68
1:C:91:ILE:HD11	1:C:106:TYR:CE2	2.29	0.68
1:B:176:THR:OG1	1:B:267:GLN:NE2	2.27	0.68
1:E:57:THR:OG1	1:E:58:ASP:N	2.27	0.68
1:C:203:ARG:NH2	1:C:271:ASP:O	2.27	0.68
1:C:221:HIS:CE1	1:C:242:ASN:HD21	2.12	0.67
1:D:41:LEU:HD23	1:D:52:GLY:HA3	1.75	0.67
1:C:225:LYS:CD	1:C:225:LYS:H	2.07	0.67
1:E:155:GLY:HA3	1:E:162:LYS:HA	1.76	0.67
1:B:169:ILE:HA	1:B:174:MET:HE1	1.77	0.67
1:C:195:MET:O	1:C:197:ALA:N	2.27	0.67
1:F:202:ARG:HG2	1:F:265:GLU:HB3	1.77	0.67
1:B:167:LYS:HG2	1:B:170:ASP:HB2	1.77	0.66
1:E:133:THR:HG21	1:E:179:LEU:HB2	1.75	0.66
1:B:150:LEU:O	1:B:166:TYR:HA	1.95	0.66
1:C:177:CYS:O	1:D:77:ARG:NH2	2.29	0.66
1:D:223:LEU:HD21	1:D:232:ILE:HD11	1.78	0.66
1:C:78:ARG:HG3	1:C:134:PRO:HA	1.77	0.66
1:F:228:GLU:HG3	1:F:230:ARG:NH1	2.06	0.66
1:E:167:LYS:HD2	1:E:170:ASP:OD2	1.95	0.66
1:E:6:VAL:HG21	1:E:8:ARG:HH21	1.62	0.65
1:B:85:ILE:HD11	1:B:210:PHE:CD2	2.32	0.65
1:B:39:ILE:HD13	1:B:54:VAL:CG1	2.24	0.65
1:A:203:ARG:HH11	1:A:266:ASN:HD21	1.45	0.65
1:A:69:LEU:HA	1:B:202:ARG:HE	1.61	0.64
1:F:114:LYS:HD2	1:F:114:LYS:C	2.16	0.64
1:A:59:GLU:HG3	1:A:60:PRO:HD2	1.79	0.64
1:F:193:ASN:OD1	1:F:194:THR:HG22	1.97	0.64
1:B:230:ARG:HH12	1:C:230:ARG:CZ	2.10	0.64
1:C:54:VAL:HG22	1:C:128:PHE:HB2	1.77	0.64
1:A:68:GLU:O	1:B:202:ARG:NH2	2.30	0.64
1:C:165:ILE:C	1:C:166:TYR:HD2	2.02	0.63
1:E:69:LEU:HA	1:F:202:ARG:NH1	2.14	0.63
1:D:75:LEU:CD1	1:D:78:ARG:CB	2.74	0.63
1:C:43:TYR:OH	1:C:48:ARG:HG2	1.98	0.63
1:F:203:ARG:HB3	1:F:264:GLY:HA3	1.79	0.63
1:F:21:THR:O	1:F:25:ARG:HG3	1.99	0.62
1:A:21:THR:O	1:A:25:ARG:HG3	1.99	0.62
1:B:107:TYR:HD1	1:B:108:ILE:N	1.97	0.62
1:E:202:ARG:CZ	1:E:271:ASP:HB2	2.29	0.62
1:E:266:ASN:OD1	1:E:267:GLN:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:HG22	1:C:97:LYS:HB2	1.80	0.62
1:B:102:ASN:OD1	1:B:103:GLN:HG2	2.00	0.62
1:F:83:ILE:HD13	1:F:168:TYR:CD2	2.34	0.62
1:C:11:HIS:HD2	1:D:15:ASP:OD1	1.82	0.61
1:F:48:ARG:O	1:F:78:ARG:NH1	2.31	0.61
1:E:38:ASP:OD2	1:E:39:ILE:N	2.33	0.61
1:F:41:LEU:HD23	1:F:52:GLY:HA3	1.83	0.61
1:B:85:ILE:HG22	1:B:127:LYS:O	2.00	0.61
1:B:225:LYS:H	1:B:225:LYS:CD	2.13	0.61
1:F:91:ILE:HG22	1:F:117:PHE:HA	1.81	0.61
1:F:200:HIS:HB3	1:F:272:MET:HG3	1.82	0.61
1:B:218:ARG:O	1:B:252:GLY:HA2	2.01	0.61
1:F:63:ILE:HD11	1:F:74:PHE:CE2	2.36	0.61
1:A:182:GLY:HA3	1:A:260:TRP:CE2	2.36	0.61
1:A:57:THR:OG1	1:A:58:ASP:N	2.33	0.61
1:A:150:LEU:O	1:A:166:TYR:HA	2.01	0.61
1:B:54:VAL:CG2	1:B:128:PHE:HB2	2.31	0.61
1:F:163:ARG:NH1	3:F:302:MPO:S1	2.74	0.61
1:B:24:LEU:HD12	1:B:230:ARG:HH21	1.66	0.60
1:C:214:ASP:OD1	1:C:217:THR:OG1	2.19	0.60
1:F:203:ARG:HE	1:F:262:MET:CE	2.13	0.60
1:B:103:GLN:OE1	1:B:103:GLN:HA	2.02	0.60
1:B:146:PHE:HE1	1:B:166:TYR:CD1	2.20	0.60
1:E:136:HIS:H	1:F:136:HIS:CD2	2.19	0.60
1:E:170:ASP:OD2	1:E:172:SER:OG	2.13	0.60
1:C:62:GLU:OE1	1:C:115:VAL:N	2.34	0.60
1:F:62:GLU:HB2	1:F:115:VAL:O	2.01	0.60
1:B:131:VAL:HB	1:B:181:MET:CE	2.31	0.60
1:E:58:ASP:HA	1:E:122:ARG:CZ	2.31	0.60
1:A:41:LEU:HD23	1:A:52:GLY:HA3	1.84	0.60
1:B:203:ARG:HH11	1:B:262:MET:HE2	1.66	0.60
1:F:203:ARG:NH1	1:F:266:ASN:OD1	2.35	0.60
1:C:135:ALA:HA	1:D:136:HIS:HD2	1.67	0.60
1:B:139:TYR:CE1	1:B:175:ASP:HB3	2.37	0.59
1:E:203:ARG:HB2	1:E:263:CYS:O	2.02	0.59
1:A:34:PHE:CE1	1:A:127:LYS:HB3	2.37	0.59
1:B:156:ASP:HA	1:B:162:LYS:HD2	1.83	0.59
1:C:92:THR:HG22	1:C:97:LYS:CB	2.32	0.59
1:F:43:TYR:OH	1:F:48:ARG:NH1	2.36	0.59
1:B:57:THR:OG1	1:B:58:ASP:N	2.35	0.59
1:B:235:PHE:H	1:B:238:GLN:NE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:THR:O	1:D:25:ARG:HG3	2.02	0.59
1:B:150:LEU:HD13	1:B:173:GLN:HE22	1.66	0.59
1:A:65:LEU:HD13	1:A:69:LEU:HD11	1.85	0.59
1:C:103:GLN:HB2	1:C:146:PHE:CD2	2.37	0.58
1:F:23:LYS:O	1:F:23:LYS:HG3	2.03	0.58
1:F:203:ARG:CB	1:F:264:GLY:HA3	2.33	0.58
1:C:58:ASP:OD1	1:C:59:GLU:N	2.36	0.58
1:E:191:SER:OG	1:E:252:GLY:N	2.37	0.58
1:C:135:ALA:HA	1:D:136:HIS:CD2	2.39	0.58
1:D:35:ASN:OD1	1:D:36:PRO:HD2	2.02	0.58
1:F:223:LEU:HD12	1:F:224:GLY:H	1.69	0.58
1:B:107:TYR:CE2	1:B:176:THR:HG22	2.39	0.58
1:F:192:TRP:CD2	1:F:251:VAL:HG22	2.39	0.58
1:A:48:ARG:O	1:A:78:ARG:NH1	2.29	0.58
1:D:182:GLY:HA3	1:D:260:TRP:CZ2	2.39	0.58
1:C:70:GLY:HA3	1:D:202:ARG:NH1	2.19	0.57
1:F:174:MET:HG2	1:F:175:ASP:H	1.70	0.57
1:D:85:ILE:HG13	1:D:127:LYS:HB2	1.86	0.57
1:F:50:ILE:HG13	1:F:78:ARG:NH1	2.19	0.57
1:A:35:ASN:OD1	1:A:36:PRO:HD2	2.05	0.57
1:D:174:MET:HG2	1:D:175:ASP:N	2.19	0.57
1:E:39:ILE:HD11	1:E:61:LEU:HB3	1.84	0.57
1:C:34:PHE:HB3	1:C:55:MET:CE	2.34	0.57
1:B:157:GLN:O	1:C:189:GLY:HA2	2.04	0.57
1:D:102:ASN:OD1	1:D:103:GLN:HG2	2.05	0.57
1:B:154:MET:HE1	3:B:302:MPO:O1	2.04	0.57
1:C:75:LEU:HD21	1:C:80:LEU:HB2	1.85	0.57
1:E:45:TYR:HE2	1:F:244:SER:HB2	1.70	0.57
1:B:182:GLY:HA3	1:B:260:TRP:CZ2	2.40	0.57
1:C:205:GLU:OE1	1:C:248:HIS:NE2	2.38	0.56
1:E:43:TYR:OH	1:E:48:ARG:HD3	2.05	0.56
1:A:165:ILE:HD11	1:A:260:TRP:HE1	1.70	0.56
1:A:136:HIS:HB2	1:B:136:HIS:HB2	1.86	0.56
1:A:279:GLU:O	1:E:233:THR:OG1	2.12	0.56
1:B:34:PHE:CD1	1:B:127:LYS:HB3	2.39	0.56
1:B:234:LEU:HD21	1:B:240:VAL:HG23	1.87	0.56
1:B:30:MET:CE	1:B:42:THR:HG23	2.36	0.56
1:A:68:GLU:O	1:B:202:ARG:NE	2.36	0.56
1:C:91:ILE:O	1:C:91:ILE:HD12	2.05	0.56
1:F:163:ARG:NH1	3:F:302:MPO:O2	2.39	0.56
1:E:64:LYS:O	1:E:65:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:GLU:OE2	1:F:248:HIS:NE2	2.38	0.56
1:C:154:MET:HG3	1:C:165:ILE:CD1	2.35	0.56
1:D:107:TYR:CE1	1:D:176:THR:HG22	2.41	0.56
1:B:150:LEU:CD1	1:B:173:GLN:HE22	2.19	0.56
1:D:203:ARG:HH11	1:D:263:CYS:CA	2.19	0.56
1:E:133:THR:CG2	1:E:179:LEU:HB2	2.35	0.56
1:E:148:THR:O	1:E:150:LEU:HD12	2.06	0.56
1:A:260:TRP:CD2	3:A:302:MPO:H72	2.41	0.55
1:B:34:PHE:HB3	1:B:55:MET:CE	2.37	0.55
1:D:182:GLY:O	1:D:259:ILE:HG23	2.06	0.55
1:E:268:THR:HG22	1:E:270:ASP:H	1.71	0.55
1:D:8:ARG:HH12	1:D:26:HIS:CD2	2.23	0.55
1:D:57:THR:OG1	1:D:58:ASP:N	2.37	0.55
1:A:203:ARG:HB2	1:A:263:CYS:O	2.06	0.55
1:C:134:PRO:O	1:C:178:GLN:NE2	2.33	0.55
1:D:218:ARG:O	1:D:252:GLY:HA2	2.06	0.55
1:C:146:PHE:HD1	1:C:146:PHE:O	1.89	0.55
1:A:69:LEU:HA	1:B:202:ARG:CZ	2.35	0.55
1:B:92:THR:O	1:B:114:LYS:NZ	2.39	0.55
1:D:33:ILE:HD13	1:D:238:GLN:HA	1.87	0.55
1:D:203:ARG:NH1	1:D:263:CYS:HA	2.19	0.55
1:F:62:GLU:OE1	1:F:116:VAL:HG12	2.06	0.55
1:C:200:HIS:ND1	1:C:203:ARG:O	2.39	0.55
1:A:242:ASN:ND2	1:A:248:HIS:HB3	2.22	0.55
1:B:203:ARG:HH11	1:B:262:MET:CE	2.19	0.55
1:D:93:ILE:HD11	1:D:141:ASN:ND2	2.22	0.55
1:E:266:ASN:OD1	1:E:268:THR:N	2.28	0.55
1:F:25:ARG:HH12	1:F:233:THR:H	1.55	0.55
1:F:121:ASP:OD1	1:F:122:ARG:N	2.39	0.55
1:A:30:MET:SD	1:A:42:THR:HG23	2.47	0.54
1:D:156:ASP:OD1	1:D:159:HIS:N	2.39	0.54
1:E:123:ASP:O	1:E:124:HIS:ND1	2.39	0.54
1:D:14:GLU:O	1:D:14:GLU:HG2	2.05	0.54
1:D:223:LEU:HD21	1:D:232:ILE:CD1	2.37	0.54
1:E:220:PHE:CD1	1:E:233:THR:HG22	2.42	0.54
1:F:137:LYS:HE2	1:F:139:TYR:CE1	2.43	0.54
1:B:171:ALA:H	1:B:180:GLN:HE22	1.55	0.54
1:C:92:THR:HA	1:C:97:LYS:HA	1.90	0.54
1:B:210:PHE:HE1	1:B:259:ILE:HG13	1.71	0.54
1:C:47:ASP:OD1	1:D:48:ARG:NH1	2.41	0.54
1:E:34:PHE:HB3	1:E:55:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:GLN:HE21	1:F:77:ARG:NH2	2.01	0.54
1:C:57:THR:OG1	1:C:58:ASP:N	2.39	0.54
1:E:139:TYR:CD1	1:E:175:ASP:HB3	2.42	0.54
1:D:210:PHE:HA	1:D:236:ASN:ND2	2.23	0.54
1:C:108:ILE:CD1	1:C:115:VAL:HG21	2.38	0.54
1:C:103:GLN:HB2	1:C:146:PHE:HD2	1.73	0.53
1:D:55:MET:HE3	1:D:127:LYS:CG	2.34	0.53
1:B:195:MET:O	1:B:197:ALA:N	2.41	0.53
1:D:219:VAL:HA	1:D:251:VAL:O	2.08	0.53
1:F:83:ILE:HD13	1:F:168:TYR:CE2	2.44	0.53
1:B:43:TYR:OH	1:B:48:ARG:NE	2.36	0.53
1:E:34:PHE:HB3	1:E:55:MET:HE2	1.89	0.53
1:D:106:TYR:CD1	1:D:142:LYS:O	2.62	0.53
1:F:207:TYR:OH	1:F:248:HIS:HD2	1.91	0.53
1:A:4:SER:HB3	1:A:40:LEU:HD23	1.91	0.53
1:A:107:TYR:CE2	1:A:176:THR:HG22	2.44	0.53
1:A:265:GLU:OE1	1:B:69:LEU:HD23	2.09	0.53
1:B:183:TYR:CE1	1:B:210:PHE:HZ	2.27	0.53
1:E:17:GLN:O	1:E:230:ARG:NH2	2.33	0.53
1:E:34:PHE:CD1	1:E:127:LYS:HB3	2.43	0.53
1:F:203:ARG:HE	1:F:262:MET:HE2	1.72	0.53
1:F:234:LEU:HD21	1:F:240:VAL:HG23	1.91	0.53
1:C:47:ASP:OD2	1:D:48:ARG:NH1	2.42	0.53
1:C:170:ASP:OD1	1:C:171:ALA:N	2.42	0.53
1:E:223:LEU:HD12	1:E:246:SER:OG	2.09	0.53
1:F:34:PHE:HB3	1:F:55:MET:HE2	1.91	0.53
1:C:136:HIS:N	1:D:136:HIS:HD2	2.02	0.52
1:D:58:ASP:HA	1:D:122:ARG:HD3	1.90	0.52
1:E:88:ALA:CB	1:E:120:GLU:HG3	2.40	0.52
1:C:208:MET:HE2	1:C:237:GLU:HA	1.91	0.52
1:E:200:HIS:CB	1:E:202:ARG:HH22	2.23	0.52
1:F:59:GLU:CD	1:F:59:GLU:H	2.12	0.52
1:F:104:ASP:OD1	1:F:146:PHE:N	2.38	0.52
1:B:5:MET:HE3	1:B:43:TYR:HD2	1.75	0.52
1:A:10:ALA:HB3	1:B:10:ALA:HB3	1.91	0.52
1:A:47:ASP:OD2	1:B:48:ARG:HD2	2.10	0.51
1:A:205:GLU:HG2	1:A:262:MET:HB2	1.91	0.51
1:B:78:ARG:HB3	1:B:134:PRO:HA	1.92	0.51
1:B:165:ILE:C	1:B:166:TYR:HD2	2.14	0.51
1:B:154:MET:CE	1:B:163:ARG:HE	2.21	0.51
1:C:179:LEU:HD12	1:C:180:GLN:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLY:HA3	1:D:162:LYS:HA	1.93	0.51
1:B:223:LEU:HD12	1:B:246:SER:OG	2.11	0.51
1:C:56:PRO:HA	1:C:61:LEU:HD12	1.91	0.51
1:C:198:HIS:CD2	1:C:248:HIS:HE2	2.28	0.51
1:F:227:ASP:O	1:F:280:LEU:HA	2.11	0.51
1:B:57:THR:HG22	1:B:125:PRO:HG3	1.91	0.51
1:D:78:ARG:HD3	1:D:134:PRO:HA	1.91	0.51
1:E:77:ARG:HH11	1:E:77:ARG:HB3	1.75	0.51
1:F:161:ASN:O	1:F:163:ARG:HD3	2.10	0.51
1:A:218:ARG:O	1:A:252:GLY:HA2	2.09	0.51
1:B:167:LYS:HD3	1:B:170:ASP:OD1	2.11	0.51
1:A:137:LYS:HE2	1:A:139:TYR:CE1	2.46	0.51
1:F:62:GLU:HB3	1:F:116:VAL:HA	1.91	0.51
1:A:107:TYR:CZ	1:A:176:THR:HG22	2.46	0.51
1:B:139:TYR:CD1	1:B:175:ASP:HB3	2.46	0.51
1:B:230:ARG:HH12	1:C:230:ARG:NE	2.09	0.51
1:C:76:GLN:O	1:C:110:MET:HG3	2.11	0.51
1:C:79:GLU:HG2	1:C:133:THR:O	2.11	0.51
1:F:163:ARG:HB3	1:F:186:LEU:HD13	1.92	0.51
1:A:54:VAL:HG12	1:A:61:LEU:HD12	1.93	0.51
1:C:225:LYS:HE2	1:C:228:GLU:HB3	1.92	0.51
1:E:11:HIS:CE1	1:F:12:SER:HB3	2.46	0.51
1:E:136:HIS:HB2	1:F:136:HIS:HB2	1.93	0.51
1:B:34:PHE:CE1	1:B:127:LYS:HB3	2.46	0.50
1:C:10:ALA:HB3	1:D:10:ALA:HB3	1.93	0.50
1:E:88:ALA:HB3	1:E:120:GLU:HG3	1.93	0.50
1:B:154:MET:SD	1:B:163:ARG:NH1	2.84	0.50
1:C:218:ARG:HH21	1:C:234:LEU:C	2.14	0.50
1:E:58:ASP:HA	1:E:122:ARG:NH1	2.26	0.50
1:E:66:SER:O	1:E:70:GLY:N	2.45	0.50
1:C:37:GLY:O	1:C:61:LEU:HD11	2.11	0.50
1:C:240:VAL:HG12	1:C:242:ASN:OD1	2.11	0.50
1:C:182:GLY:O	1:C:259:ILE:HG23	2.12	0.50
1:D:31:GLU:O	1:D:238:GLN:HG2	2.12	0.50
1:E:170:ASP:OD1	1:E:171:ALA:N	2.44	0.50
1:F:91:ILE:HD11	1:F:106:TYR:CD2	2.46	0.50
1:A:2:SER:HB3	1:A:38:ASP:OD1	2.11	0.50
1:C:225:LYS:H	1:C:225:LYS:HD2	1.75	0.50
1:D:59:GLU:HG3	1:D:60:PRO:CD	2.42	0.50
1:A:36:PRO:N	1:A:55:MET:HE3	2.26	0.50
1:A:110:MET:HG2	1:A:111:GLY:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:HB3	1:C:55:MET:HE2	1.94	0.50
1:F:90:ALA:O	1:F:118:THR:HG22	2.11	0.50
1:B:210:PHE:CE1	1:B:259:ILE:HG13	2.46	0.49
1:C:12:SER:HB3	1:C:15:ASP:CG	2.32	0.49
1:F:133:THR:HG21	1:F:178:GLN:HG3	1.93	0.49
1:A:170:ASP:OD2	1:A:172:SER:OG	2.29	0.49
1:F:210:PHE:HA	1:F:236:ASN:OD1	2.13	0.49
1:D:203:ARG:NE	1:D:262:MET:HG2	2.27	0.49
1:F:203:ARG:NH2	1:F:268:THR:O	2.44	0.49
1:A:16:ILE:HG22	1:A:19:TYR:CE2	2.47	0.49
1:D:82:ILE:HD13	1:D:117:PHE:HE2	1.77	0.49
1:E:200:HIS:HB2	1:E:202:ARG:HH22	1.78	0.49
1:F:63:ILE:O	1:F:63:ILE:HG13	2.11	0.49
1:F:75:LEU:HD12	1:F:78:ARG:HB2	1.94	0.49
1:B:218:ARG:NH2	1:B:235:PHE:CD2	2.79	0.49
1:C:225:LYS:HD3	1:C:228:GLU:O	2.13	0.49
1:D:166:TYR:HB2	1:D:183:TYR:HB3	1.95	0.49
1:F:39:ILE:HG23	1:F:54:VAL:HG12	1.94	0.49
1:B:183:TYR:HE1	1:B:210:PHE:CZ	2.30	0.49
1:A:19:TYR:CD1	1:A:23:LYS:NZ	2.54	0.49
1:C:39:ILE:HG23	1:C:54:VAL:HG12	1.94	0.49
1:B:161:ASN:HB2	1:B:163:ARG:HH22	1.77	0.49
1:E:198:HIS:HB3	1:E:272:MET:HE3	1.94	0.49
1:A:99:ALA:O	1:A:143:LYS:NZ	2.42	0.48
1:B:170:ASP:H	1:B:174:MET:HE3	1.78	0.48
1:D:62:GLU:HG3	1:D:115:VAL:O	2.13	0.48
1:E:200:HIS:CB	1:E:202:ARG:NH2	2.74	0.48
1:E:203:ARG:CB	1:E:264:GLY:HA3	2.43	0.48
1:F:223:LEU:HD12	1:F:246:SER:OG	2.13	0.48
1:A:157:GLN:O	1:E:189:GLY:HA2	2.13	0.48
1:A:205:GLU:OE2	1:A:248:HIS:CE1	2.66	0.48
1:B:21:THR:HG21	1:C:228:GLU:HA	1.94	0.48
1:F:11:HIS:NE2	1:F:27:GLU:OE2	2.46	0.48
1:F:137:LYS:HD3	1:F:139:TYR:CZ	2.48	0.48
1:F:167:LYS:HG3	1:F:170:ASP:CB	2.43	0.48
1:B:154:MET:HE1	1:B:163:ARG:NE	2.12	0.48
1:A:156:ASP:OD1	1:A:159:HIS:N	2.42	0.48
1:F:64:LYS:O	1:F:65:LEU:HD23	2.13	0.48
1:C:225:LYS:H	1:C:225:LYS:HD3	1.76	0.48
1:F:56:PRO:HG2	1:F:128:PHE:CE2	2.44	0.48
1:B:117:PHE:HB3	1:B:128:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:LEU:CA	1:F:202:ARG:HH12	2.26	0.48
1:B:110:MET:HG2	1:B:111:GLY:N	2.28	0.48
1:C:115:VAL:HG13	1:C:115:VAL:O	2.12	0.48
1:F:91:ILE:HD12	1:F:91:ILE:O	2.13	0.48
1:C:41:LEU:HD23	1:C:52:GLY:HA3	1.96	0.48
1:A:53:GLY:HA2	1:A:128:PHE:O	2.13	0.47
1:C:266:ASN:ND2	1:C:268:THR:HG23	2.24	0.47
1:E:29:LEU:CD2	1:E:31:GLU:HG2	2.44	0.47
1:F:39:ILE:HD13	1:F:63:ILE:HG22	1.96	0.47
1:F:82:ILE:HD13	1:F:106:TYR:HB3	1.96	0.47
1:B:144:LEU:HD21	1:B:174:MET:SD	2.54	0.47
1:C:82:ILE:HD13	1:C:117:PHE:HE2	1.78	0.47
1:F:63:ILE:HD11	1:F:74:PHE:CZ	2.49	0.47
1:F:94:ASP:HA	1:F:114:LYS:HE3	1.96	0.47
1:C:203:ARG:HB2	1:C:263:CYS:O	2.15	0.47
1:C:214:ASP:OD1	1:C:214:ASP:N	2.46	0.47
1:D:207:TYR:HH	1:D:248:HIS:HD1	1.58	0.47
1:E:107:TYR:O	1:E:108:ILE:HD13	2.14	0.47
1:E:200:HIS:ND1	1:E:203:ARG:O	2.48	0.47
1:C:91:ILE:HA	1:C:116:VAL:O	2.14	0.47
1:D:203:ARG:HH21	1:D:266:ASN:C	2.14	0.47
1:E:67:THR:C	1:E:70:GLY:H	2.18	0.47
1:F:91:ILE:HA	1:F:116:VAL:O	2.14	0.47
1:F:205:GLU:HG2	1:F:262:MET:HB2	1.96	0.47
1:B:171:ALA:N	1:B:180:GLN:HE22	2.11	0.47
1:C:144:LEU:HD22	1:C:168:TYR:O	2.14	0.47
1:A:34:PHE:CD1	1:A:127:LYS:HB3	2.50	0.47
1:A:83:ILE:HG13	1:A:181:MET:HE3	1.97	0.47
1:A:137:LYS:HE2	1:A:139:TYR:CZ	2.49	0.47
1:A:163:ARG:HD3	1:A:184:THR:CG2	2.44	0.47
1:A:182:GLY:HA3	1:A:260:TRP:CZ2	2.50	0.47
1:B:29:LEU:HD23	1:B:31:GLU:HG2	1.96	0.47
1:B:170:ASP:H	1:B:174:MET:CE	2.28	0.47
1:C:150:LEU:HG	1:C:151:ALA:N	2.30	0.47
1:C:166:TYR:N	1:C:166:TYR:CD2	2.83	0.47
1:D:115:VAL:HG12	1:D:117:PHE:CE1	2.50	0.47
1:E:29:LEU:CD1	1:E:234:LEU:HD22	2.44	0.47
1:E:179:LEU:HD11	1:E:181:MET:HG3	1.97	0.47
1:A:142:LYS:HZ1	1:A:174:MET:CB	2.22	0.47
1:C:29:LEU:CD2	1:C:31:GLU:HG2	2.45	0.47
1:D:19:TYR:HE1	1:D:27:GLU:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LEU:HD23	1:C:31:GLU:HG2	1.97	0.47
1:A:202:ARG:HB2	1:A:266:ASN:ND2	2.29	0.47
1:B:29:LEU:CD2	1:B:31:GLU:HG2	2.45	0.47
1:B:226:PRO:O	1:B:279:GLU:HA	2.15	0.47
1:F:73:PHE:CD2	1:F:113:GLN:HA	2.50	0.47
1:F:210:PHE:HD2	1:F:211:ASN:ND2	2.10	0.47
1:F:212:PHE:HB3	1:F:217:THR:HB	1.96	0.47
1:A:228:GLU:HG3	1:A:230:ARG:HH12	1.80	0.46
1:B:146:PHE:HE1	1:B:166:TYR:HD1	1.61	0.46
1:C:92:THR:OG1	1:C:116:VAL:CG1	2.60	0.46
1:C:220:PHE:N	1:C:251:VAL:O	2.30	0.46
1:E:40:LEU:O	1:E:52:GLY:HA3	2.15	0.46
1:E:136:HIS:H	1:F:136:HIS:HD2	1.60	0.46
1:F:25:ARG:NH1	1:F:233:THR:H	2.13	0.46
1:E:179:LEU:HD12	1:E:180:GLN:N	2.30	0.46
1:E:195:MET:HB3	1:E:196:PRO:CD	2.44	0.46
1:F:226:PRO:O	1:F:279:GLU:HA	2.16	0.46
1:B:35:ASN:OD1	1:B:36:PRO:HD2	2.15	0.46
1:A:277:MET:HG3	1:E:216:GLU:HB3	1.98	0.46
1:B:6:VAL:HG22	1:B:42:THR:HG22	1.98	0.46
1:F:200:HIS:NE2	1:F:205:GLU:OE2	2.48	0.46
1:D:205:GLU:HG2	1:D:262:MET:HB2	1.98	0.46
1:C:82:ILE:HD13	1:C:117:PHE:CE2	2.51	0.46
1:A:279:GLU:N	1:E:218:ARG:NH1	2.52	0.46
1:B:5:MET:HA	1:B:41:LEU:O	2.15	0.46
1:D:35:ASN:O	1:D:55:MET:HG2	2.16	0.46
1:E:77:ARG:HH21	1:F:267:GLN:HE21	1.64	0.46
1:F:34:PHE:HE2	1:F:208:MET:HE3	1.80	0.46
1:F:56:PRO:HA	1:F:61:LEU:HD12	1.98	0.46
1:F:195:MET:O	1:F:197:ALA:N	2.49	0.46
1:C:165:ILE:O	1:C:166:TYR:HD2	1.99	0.46
1:C:198:HIS:HB2	1:C:272:MET:HB2	1.98	0.46
1:D:231:HIS:NE2	1:F:229:THR:OG1	2.41	0.46
1:A:110:MET:HE1	1:A:136:HIS:C	2.37	0.45
1:D:21:THR:HG23	1:F:230:ARG:NH1	2.31	0.45
1:F:260:TRP:CE2	3:F:302:MPO:H72	2.51	0.45
1:B:21:THR:N	1:C:228:GLU:OE2	2.45	0.45
1:B:96:ARG:NH1	1:B:96:ARG:HA	2.29	0.45
1:B:107:TYR:CD1	1:B:108:ILE:N	2.80	0.45
1:B:189:GLY:HA2	1:C:157:GLN:O	2.15	0.45
1:B:202:ARG:C	1:B:203:ARG:HG2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PHE:HE1	1:C:259:ILE:HG13	1.81	0.45
1:D:32:LYS:HD2	1:D:34:PHE:O	2.16	0.45
1:B:2:SER:HB2	1:B:38:ASP:OD1	2.16	0.45
1:C:165:ILE:C	1:C:166:TYR:CD2	2.86	0.45
1:C:179:LEU:HD12	1:C:180:GLN:H	1.81	0.45
1:C:187:GLU:O	1:C:190:SER:HB2	2.16	0.45
1:F:59:GLU:O	1:F:60:PRO:C	2.55	0.45
1:F:61:LEU:O	1:F:117:PHE:N	2.37	0.45
1:F:158:GLN:O	1:F:158:GLN:HG3	2.15	0.45
1:B:11:HIS:HB3	1:B:15:ASP:HB2	1.98	0.45
1:C:19:TYR:HE2	1:C:27:GLU:HG3	1.81	0.45
1:C:216:GLU:N	1:C:216:GLU:OE1	2.49	0.45
1:D:3:PHE:HD1	1:D:39:ILE:HB	1.80	0.45
1:A:19:TYR:CB	1:A:23:LYS:HZ1	2.15	0.45
1:C:224:GLY:O	1:C:247:ILE:HG12	2.16	0.45
1:D:218:ARG:NH2	1:F:279:GLU:O	2.48	0.45
1:F:62:GLU:CB	1:F:116:VAL:HA	2.46	0.45
1:A:91:ILE:HD11	1:A:106:TYR:CD2	2.52	0.45
1:C:30:MET:SD	1:C:42:THR:HG23	2.57	0.45
1:C:71:VAL:HB	1:C:76:GLN:OE1	2.16	0.45
1:D:194:THR:HG22	1:D:194:THR:O	2.15	0.45
1:E:152:LYS:O	1:E:165:ILE:HG22	2.17	0.45
1:E:203:ARG:HH21	1:E:262:MET:CE	2.29	0.45
1:B:200:HIS:ND1	1:B:203:ARG:O	2.50	0.45
1:D:192:TRP:CD2	1:D:251:VAL:HG12	2.51	0.45
1:F:214:ASP:OD1	1:F:215:PRO:HD3	2.17	0.45
1:B:21:THR:HB	1:C:280:LEU:CD1	2.47	0.45
1:B:98:ASP:OD1	1:B:143:LYS:NZ	2.49	0.45
1:D:42:THR:HB	1:D:51:PHE:CE1	2.51	0.45
1:D:179:LEU:HD12	1:D:180:GLN:N	2.32	0.45
1:D:227:ASP:OD1	1:D:228:GLU:N	2.50	0.45
1:E:3:PHE:CZ	1:E:65:LEU:HD21	2.51	0.45
1:A:85:ILE:HA	1:A:103:GLN:NE2	2.32	0.45
1:A:221:HIS:CD2	1:A:240:VAL:HG11	2.52	0.45
3:B:302:MPO:H42	3:B:302:MPO:H11	1.98	0.45
1:D:92:THR:HG22	1:D:97:LYS:HB2	1.98	0.45
1:B:48:ARG:O	1:B:78:ARG:NH2	2.49	0.44
1:F:129:TYR:CE1	1:F:208:MET:HG3	2.53	0.44
1:C:34:PHE:CD1	1:C:127:LYS:HB3	2.52	0.44
1:D:129:TYR:CE2	1:D:208:MET:HG3	2.52	0.44
1:A:6:VAL:HG22	1:A:42:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LYS:HE2	1:B:116:VAL:CB	2.41	0.44
1:C:92:THR:HG22	1:C:97:LYS:CG	2.47	0.44
1:D:73:PHE:CD2	1:D:113:GLN:HA	2.53	0.44
1:D:145:PRO:HD2	1:D:148:THR:OG1	2.17	0.44
1:A:23:LYS:HB3	1:A:23:LYS:HE3	1.20	0.44
1:A:102:ASN:OD1	1:A:103:GLN:HG2	2.17	0.44
1:B:231:HIS:NE2	1:C:229:THR:HG23	2.33	0.44
1:C:210:PHE:CE1	1:C:259:ILE:HG13	2.52	0.44
1:E:6:VAL:HG21	1:E:8:ARG:NH2	2.31	0.44
1:E:214:ASP:OD1	1:E:215:PRO:HD2	2.17	0.44
1:F:92:THR:HG22	1:F:97:LYS:CD	2.48	0.44
1:A:19:TYR:HB3	1:A:23:LYS:NZ	2.15	0.44
1:A:277:MET:HE2	1:E:216:GLU:O	2.18	0.44
1:B:69:LEU:N	1:B:69:LEU:HD12	2.33	0.44
1:C:179:LEU:O	1:C:180:GLN:HG2	2.18	0.44
1:E:102:ASN:OD1	1:E:103:GLN:HG2	2.18	0.44
1:E:208:MET:HG2	1:E:239:ALA:HB2	1.99	0.44
1:A:68:GLU:O	1:B:202:ARG:CZ	2.65	0.44
1:A:129:TYR:CE1	1:A:208:MET:HG3	2.52	0.44
1:E:2:SER:OG	1:E:3:PHE:N	2.51	0.44
1:F:174:MET:HG2	1:F:175:ASP:N	2.32	0.44
1:A:75:LEU:HD21	1:A:80:LEU:HB2	2.00	0.44
1:B:203:ARG:NH2	1:B:271:ASP:O	2.51	0.44
1:B:224:GLY:HA2	1:B:245:TRP:HZ3	1.82	0.44
1:C:54:VAL:HG21	1:C:117:PHE:CG	2.53	0.44
1:F:107:TYR:O	1:F:108:ILE:HD13	2.17	0.44
1:A:12:SER:OG	1:A:14:GLU:HB2	2.18	0.44
1:A:39:ILE:HG12	1:A:54:VAL:HG13	1.98	0.44
1:B:91:ILE:HD11	1:B:106:TYR:CD1	2.53	0.44
1:C:75:LEU:CD2	1:C:80:LEU:HB2	2.46	0.44
1:D:82:ILE:HD13	1:D:117:PHE:CE2	2.52	0.44
1:A:73:PHE:CD2	1:A:113:GLN:HA	2.53	0.43
1:F:49:MET:HE1	1:F:206:THR:HB	2.00	0.43
1:D:51:PHE:CD2	1:D:206:THR:HG21	2.53	0.43
1:D:93:ILE:HD11	1:D:141:ASN:HD22	1.81	0.43
1:D:134:PRO:HD2	1:D:178:GLN:NE2	2.33	0.43
1:D:234:LEU:HD21	1:D:240:VAL:HG23	1.99	0.43
1:E:272:MET:HE3	1:E:272:MET:HA	2.00	0.43
1:A:178:GLN:HE21	1:A:264:GLY:N	2.17	0.43
1:B:30:MET:SD	1:B:42:THR:HG23	2.58	0.43
1:F:209:TYR:HB3	1:F:212:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:HIS:HE1	1:C:242:ASN:ND2	2.08	0.43
1:D:34:PHE:CE2	1:D:85:ILE:HD11	2.53	0.43
1:F:225:LYS:HB3	1:F:225:LYS:HZ3	1.80	0.43
1:C:78:ARG:HG3	1:C:134:PRO:CA	2.45	0.43
1:E:48:ARG:HD2	1:F:265:GLU:HB2	1.99	0.43
1:F:226:PRO:HG3	1:F:275:VAL:HG11	2.01	0.43
1:A:16:ILE:O	1:A:19:TYR:HB2	2.19	0.43
1:A:77:ARG:NE	1:B:266:ASN:HA	2.34	0.43
1:A:270:ASP:OD2	1:A:270:ASP:N	2.42	0.43
1:B:85:ILE:CG2	1:B:127:LYS:HB2	2.49	0.43
1:B:218:ARG:NH2	1:B:235:PHE:CE2	2.83	0.43
1:C:7:THR:O	1:C:8:ARG:NH1	2.52	0.43
1:E:70:GLY:HA3	1:F:202:ARG:HH22	1.84	0.43
1:F:139:TYR:HD1	1:F:139:TYR:HA	1.73	0.43
1:F:156:ASP:OD1	1:F:159:HIS:N	2.47	0.43
1:A:200:HIS:CE1	1:A:203:ARG:O	2.72	0.43
1:A:202:ARG:HD2	1:B:68:GLU:O	2.17	0.43
1:B:92:THR:HA	1:B:97:LYS:HA	1.99	0.43
1:C:15:ASP:OD1	1:D:11:HIS:HD2	2.02	0.43
1:C:266:ASN:HD21	1:C:268:THR:CG2	2.26	0.43
1:E:162:LYS:N	1:E:190:SER:OG	2.51	0.43
1:F:11:HIS:CE1	1:F:27:GLU:OE2	2.72	0.43
1:B:68:GLU:HB2	1:B:69:LEU:HD12	2.01	0.43
1:B:228:GLU:OE1	1:C:20:ASP:HB2	2.18	0.43
1:B:222:PHE:HB2	1:B:249:CYS:HB2	2.01	0.43
1:E:77:ARG:NH2	1:F:267:GLN:HE21	2.17	0.43
1:E:198:HIS:HB3	1:E:272:MET:CE	2.48	0.43
1:E:203:ARG:HB2	1:E:264:GLY:HA3	2.00	0.43
1:F:202:ARG:HE	1:F:202:ARG:HB2	1.22	0.43
1:A:82:ILE:HD13	1:A:117:PHE:HE1	1.84	0.43
1:C:69:LEU:HD13	1:D:265:GLU:OE1	2.18	0.43
1:E:40:LEU:O	1:E:41:LEU:HD23	2.19	0.43
1:E:78:ARG:HG2	1:E:134:PRO:HA	1.99	0.43
1:E:221:HIS:CG	1:E:240:VAL:HG11	2.53	0.43
1:F:145:PRO:O	1:F:148:THR:HG22	2.19	0.43
1:B:21:THR:HG23	1:C:228:GLU:HG3	2.01	0.42
1:B:62:GLU:HG3	1:B:115:VAL:O	2.19	0.42
1:B:146:PHE:HE1	1:B:166:TYR:CE1	2.36	0.42
1:E:165:ILE:HD12	1:E:183:TYR:O	2.19	0.42
1:F:208:MET:HE2	1:F:237:GLU:HA	2.01	0.42
1:A:266:ASN:OD1	1:A:268:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:HD3	1:B:202:ARG:HA	1.57	0.42
1:E:23:LYS:O	1:E:27:GLU:HB2	2.19	0.42
1:F:184:THR:HB	1:F:258:PHE:CE1	2.54	0.42
1:C:31:GLU:O	1:C:238:GLN:HG2	2.20	0.42
1:A:28:PHE:CD2	1:A:223:LEU:HD21	2.53	0.42
1:B:166:TYR:N	1:B:166:TYR:CD2	2.88	0.42
1:D:3:PHE:CD1	1:D:39:ILE:HB	2.54	0.42
1:D:24:LEU:HD23	1:D:24:LEU:HA	1.81	0.42
1:D:25:ARG:HG2	1:D:232:ILE:HG23	2.00	0.42
1:F:25:ARG:O	1:F:29:LEU:HB3	2.19	0.42
1:F:202:ARG:NH2	1:F:266:ASN:ND2	2.67	0.42
1:A:152:LYS:HB3	1:A:165:ILE:CG2	2.49	0.42
1:A:227:ASP:OD2	1:A:280:LEU:HD13	2.19	0.42
1:C:136:HIS:CG	1:D:177:CYS:HB3	2.54	0.42
1:D:16:ILE:HA	1:D:19:TYR:CE2	2.54	0.42
1:D:25:ARG:O	1:D:29:LEU:HB3	2.18	0.42
1:D:39:ILE:HG23	1:D:54:VAL:HG22	2.01	0.42
1:D:169:ILE:HA	1:D:174:MET:HE3	2.00	0.42
1:B:209:TYR:CE2	1:B:219:VAL:HG11	2.55	0.42
1:D:36:PRO:HA	1:D:55:MET:HG3	2.01	0.42
1:A:152:LYS:HB3	1:A:165:ILE:HG23	2.02	0.42
1:A:44:THR:O	1:A:48:ARG:HA	2.19	0.42
1:C:133:THR:CG2	1:C:178:GLN:HG3	2.50	0.42
1:D:135:ALA:HB1	1:D:177:CYS:SG	2.60	0.42
1:E:16:ILE:HG22	1:E:19:TYR:CE2	2.54	0.42
1:F:202:ARG:CG	1:F:265:GLU:HB3	2.48	0.42
1:B:106:TYR:CE1	1:B:143:LYS:HB2	2.55	0.42
1:E:184:THR:HB	1:E:258:PHE:CE1	2.54	0.42
1:F:202:ARG:HH11	1:F:202:ARG:HD2	1.31	0.42
1:A:12:SER:HB2	1:B:11:HIS:HE1	1.85	0.42
1:A:40:LEU:O	1:A:52:GLY:HA3	2.20	0.42
1:A:91:ILE:HG22	1:A:117:PHE:HA	2.02	0.42
1:A:201:ALA:O	1:B:48:ARG:NH2	2.53	0.42
1:D:11:HIS:CE1	1:D:27:GLU:OE1	2.73	0.42
1:E:203:ARG:C	1:E:244:SER:HG	2.23	0.42
1:B:107:TYR:CD1	1:B:107:TYR:C	2.93	0.41
1:C:217:THR:C	1:C:218:ARG:HG2	2.41	0.41
1:D:139:TYR:CE1	1:D:175:ASP:HB3	2.55	0.41
1:D:200:HIS:CE1	1:D:203:ARG:O	2.73	0.41
1:D:229:THR:HG23	1:F:231:HIS:NE2	2.35	0.41
1:E:107:TYR:CZ	1:E:176:THR:HG22	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:THR:HG22	1:B:116:VAL:HG12	2.02	0.41
1:B:234:LEU:HD21	1:B:240:VAL:CG2	2.50	0.41
1:C:92:THR:CG2	1:C:97:LYS:HB2	2.48	0.41
1:D:8:ARG:NH1	1:D:26:HIS:O	2.53	0.41
1:A:29:LEU:HD12	1:A:239:ALA:O	2.19	0.41
1:A:178:GLN:HG2	1:A:264:GLY:O	2.20	0.41
1:B:69:LEU:CD2	1:B:78:ARG:HH11	2.33	0.41
1:E:273:ASP:OD1	1:E:273:ASP:N	2.54	0.41
1:F:94:ASP:CA	1:F:114:LYS:HE3	2.49	0.41
1:D:65:LEU:HD13	1:D:69:LEU:HD11	2.02	0.41
1:D:200:HIS:ND1	1:D:203:ARG:O	2.53	0.41
1:D:207:TYR:O	1:D:239:ALA:HA	2.19	0.41
1:F:101:SER:O	1:F:104:ASP:HB2	2.20	0.41
1:B:85:ILE:HG21	1:B:85:ILE:HD13	1.77	0.41
1:B:192:TRP:CD2	1:B:251:VAL:HG12	2.54	0.41
1:A:150:LEU:HD13	1:A:167:LYS:HG3	2.02	0.41
1:B:57:THR:HB	1:B:122:ARG:HG3	2.03	0.41
1:C:107:TYR:CZ	1:C:176:THR:HG22	2.56	0.41
1:F:29:LEU:HD12	1:F:239:ALA:O	2.20	0.41
1:F:218:ARG:O	1:F:252:GLY:HA2	2.20	0.41
1:B:114:LYS:HZ2	1:B:114:LYS:HG3	1.65	0.41
1:F:39:ILE:HG12	1:F:54:VAL:HG12	2.03	0.41
1:C:78:ARG:HG3	1:C:133:THR:C	2.41	0.41
1:C:78:ARG:HH21	1:C:78:ARG:HD3	1.67	0.41
1:E:136:HIS:N	1:F:136:HIS:HD2	2.17	0.41
1:A:220:PHE:HB2	1:A:251:VAL:CG2	2.51	0.41
1:B:202:ARG:HD3	1:B:202:ARG:HH11	1.61	0.41
1:C:90:ALA:HB3	1:C:97:LYS:NZ	2.36	0.41
1:D:55:MET:HE2	1:D:125:PRO:HG2	2.03	0.41
1:D:191:SER:OG	1:D:252:GLY:O	2.28	0.41
1:D:211:ASN:N	1:D:236:ASN:HD21	2.19	0.41
1:E:87:GLY:N	1:E:126:ALA:HA	2.36	0.41
1:F:91:ILE:HG21	1:F:117:PHE:CD2	2.56	0.41
1:B:8:ARG:NH1	1:B:26:HIS:O	2.50	0.41
1:C:43:TYR:CZ	1:C:48:ARG:HG2	2.56	0.41
1:D:110:MET:HG2	1:D:111:GLY:N	2.33	0.41
1:E:107:TYR:CE1	1:E:176:THR:HG22	2.56	0.41
1:F:78:ARG:HG2	1:F:134:PRO:HA	2.01	0.41
1:F:143:LYS:O	1:F:145:PRO:HD3	2.21	0.41
1:B:60:PRO:HB2	1:B:116:VAL:HG21	2.02	0.40
1:B:156:ASP:CA	1:B:162:LYS:HD2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ALA:HB1	1:F:177:CYS:SG	2.61	0.40
1:B:169:ILE:CG2	1:B:176:THR:HG21	2.51	0.40
1:C:48:ARG:NH1	1:D:47:ASP:OD2	2.45	0.40
1:C:164:THR:HG1	1:C:166:TYR:HE2	1.69	0.40
1:D:41:LEU:HD23	1:D:52:GLY:CA	2.49	0.40
1:E:156:ASP:OD2	1:E:159:HIS:N	2.50	0.40
1:F:55:MET:HE2	1:F:55:MET:HB2	1.91	0.40
1:A:192:TRP:CD2	1:A:251:VAL:HG12	2.56	0.40
1:B:24:LEU:HD23	1:B:24:LEU:HA	1.75	0.40
1:B:169:ILE:HA	1:B:174:MET:CE	2.46	0.40
1:B:235:PHE:N	1:B:238:GLN:NE2	2.69	0.40
1:C:34:PHE:CE2	1:C:85:ILE:HD11	2.56	0.40
1:C:198:HIS:CD2	1:C:248:HIS:NE2	2.88	0.40
1:E:29:LEU:HD12	1:E:234:LEU:HD22	2.04	0.40
1:A:127:LYS:NZ	1:A:237:GLU:OE2	2.46	0.40
1:D:8:ARG:NH1	1:D:26:HIS:CE1	2.89	0.40
1:D:36:PRO:HA	1:D:55:MET:CG	2.51	0.40
1:F:65:LEU:HD23	1:F:65:LEU:HA	1.96	0.40
1:F:115:VAL:O	1:F:115:VAL:HG13	2.21	0.40
1:A:78:ARG:HG2	1:A:134:PRO:HA	2.04	0.40
1:A:178:GLN:HE21	1:A:264:GLY:H	1.68	0.40
1:A:214:ASP:OD1	1:A:215:PRO:N	2.54	0.40
1:B:114:LYS:HD2	1:B:115:VAL:N	2.36	0.40
1:E:91:ILE:HG22	1:E:93:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	277/289 (96%)	270 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	273/289 (94%)	261 (96%)	11 (4%)	1 (0%)	34 66
1	C	277/289 (96%)	268 (97%)	8 (3%)	1 (0%)	34 66
1	D	257/289 (89%)	250 (97%)	7 (3%)	0	100 100
1	E	272/289 (94%)	264 (97%)	8 (3%)	0	100 100
1	F	270/289 (93%)	262 (97%)	8 (3%)	0	100 100
All	All	1626/1734 (94%)	1575 (97%)	49 (3%)	2 (0%)	51 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ALA
1	C	196	PRO

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	243/253 (96%)	233 (96%)	10 (4%)	30 64
1	B	240/253 (95%)	226 (94%)	14 (6%)	20 50
1	C	243/253 (96%)	234 (96%)	9 (4%)	34 68
1	D	227/253 (90%)	220 (97%)	7 (3%)	40 74
1	E	241/253 (95%)	234 (97%)	7 (3%)	42 76
1	F	240/253 (95%)	225 (94%)	15 (6%)	18 46
All	All	1434/1518 (94%)	1372 (96%)	62 (4%)	29 62

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	58	ASP
1	A	92	THR
1	A	106	TYR

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Mol	Chain	Res	Type
1	A	122	ARG
1	A	163	ARG
1	A	202	ARG
1	A	248	HIS
1	A	249	CYS
1	A	272	MET
1	B	4	SER
1	B	8	ARG
1	B	96	ARG
1	B	106	TYR
1	B	107	TYR
1	B	167	LYS
1	B	174	MET
1	B	190	SER
1	B	194	THR
1	B	202	ARG
1	B	204	MET
1	B	225	LYS
1	B	230	ARG
1	B	263	CYS
1	C	14	GLU
1	C	64	LYS
1	C	106	TYR
1	C	146	PHE
1	C	163	ARG
1	C	167	LYS
1	C	181	MET
1	C	225	LYS
1	C	248	HIS
1	D	51	PHE
1	D	106	TYR
1	D	142	LYS
1	D	204	MET
1	D	223	LEU
1	D	228	GLU
1	D	248	HIS
1	E	59	GLU
1	E	106	TYR
1	E	133	THR
1	E	164	THR
1	E	248	HIS
1	E	263	CYS

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Mol	Chain	Res	Type
1	E	273	ASP
1	F	55	MET
1	F	61	LEU
1	F	72	ASP
1	F	83	ILE
1	F	97	LYS
1	F	102	ASN
1	F	106	TYR
1	F	114	LYS
1	F	202	ARG
1	F	214	ASP
1	F	248	HIS
1	F	249	CYS
1	F	263	CYS
1	F	269	TYR
1	F	273	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	178	GLN
1	A	242	ASN
1	B	173	GLN
1	B	180	GLN
1	B	238	GLN
1	B	248	HIS
1	C	11	HIS
1	C	84	ASN
1	C	221	HIS
1	C	266	ASN
1	D	11	HIS
1	D	84	ASN
1	D	136	HIS
1	D	157	GLN
1	D	236	ASN
1	E	84	ASN
1	E	157	GLN
1	E	267	GLN
1	F	136	HIS
1	F	267	GLN
1	F	274	GLN

### 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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MPO	E	302	-	13,13,13	0.67	1 (7%)	17,17,17	0.57	0
3	MPO	B	302	-	13,13,13	1.06	1 (7%)	17,17,17	1.13	1 (5%)
3	MPO	F	302	-	13,13,13	0.61	1 (7%)	17,17,17	0.93	2 (11%)
3	MPO	A	302	-	13,13,13	1.08	1 (7%)	17,17,17	1.55	2 (11%)

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	MPO	E	302	-	-	0/7/15/15	0/1/1/1
3	MPO	B	302	-	-	1/7/15/15	0/1/1/1
3	MPO	F	302	-	-	3/7/15/15	0/1/1/1
3	MPO	A	302	-	-	2/7/15/15	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	MPO	O1-S1	3.70	1.55	1.45
3	B	302	MPO	O2-S1	3.63	1.55	1.45
3	E	302	MPO	O3-S1	2.33	1.55	1.47
3	F	302	MPO	O3-S1	2.13	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	MPO	O1-S1-C1	-4.58	101.40	106.92
3	A	302	MPO	O3-S1-O2	3.85	120.69	111.27
3	B	302	MPO	O3-S1-O1	3.50	119.82	111.27
3	F	302	MPO	O3-S1-C1	-2.36	101.95	105.77
3	F	302	MPO	O2-S1-O1	2.17	121.47	113.95

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	302	MPO	C2-C3-N1-C4
3	F	302	MPO	C2-C3-N1-C7
3	A	302	MPO	C2-C1-S1-O1
3	A	302	MPO	C2-C1-S1-O2
3	B	302	MPO	C1-C2-C3-N1
3	F	302	MPO	C2-C1-S1-O2

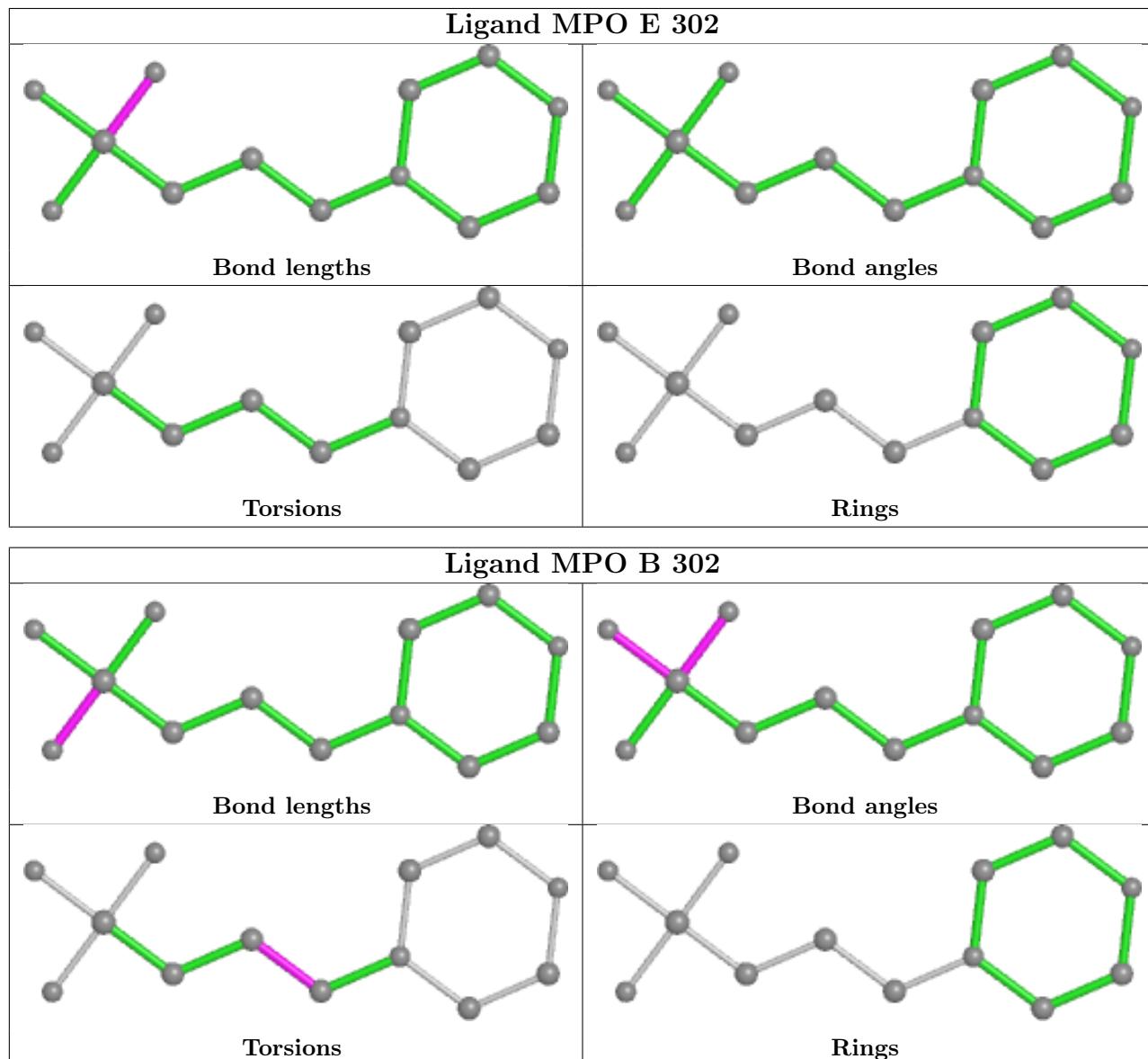
There are no ring outliers.

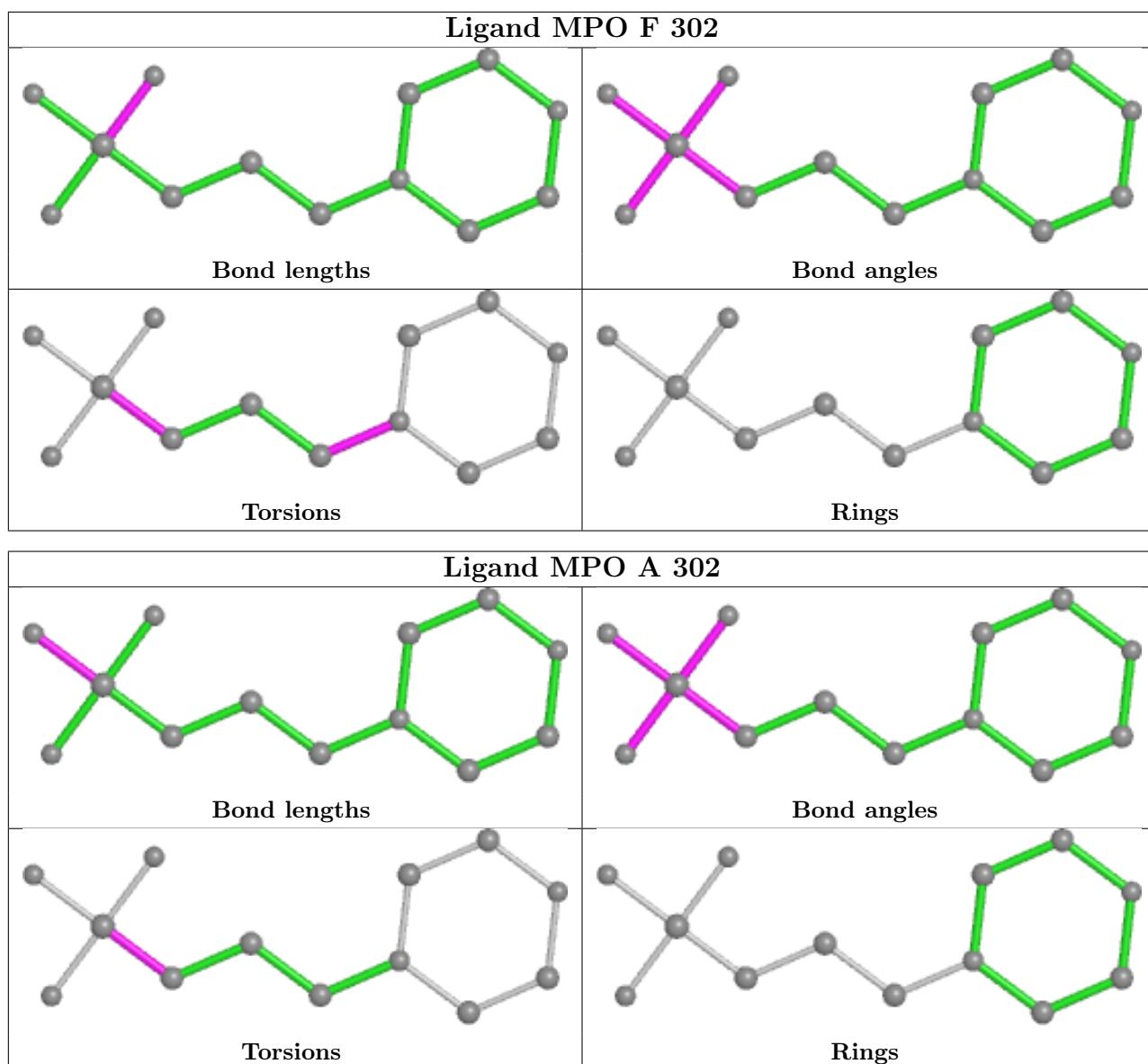
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	MPO	2	0
3	F	302	MPO	4	0
3	A	302	MPO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

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%)	-0.07	4 (1%) 75 70	46, 68, 113, 171	0
1	B	276/289 (95%)	0.28	14 (5%) 28 19	30, 81, 129, 175	0
1	C	279/289 (96%)	0.38	21 (7%) 14 8	49, 88, 132, 160	0
1	D	261/289 (90%)	-0.09	1 (0%) 92 91	41, 73, 110, 164	0
1	E	276/289 (95%)	0.29	13 (4%) 31 22	42, 78, 137, 226	0
1	F	276/289 (95%)	0.23	12 (4%) 35 25	44, 80, 131, 200	0
All	All	1647/1734 (94%)	0.17	65 (3%) 39 29	30, 77, 130, 226	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	ALA	4.9
1	C	280	LEU	4.7
1	C	81	GLY	4.6
1	F	277	MET	4.6
1	B	153	PRO	4.4
1	C	277	MET	4.2
1	E	122	ARG	4.1
1	B	2	SER	4.0
1	E	195	MET	3.8
1	E	270	ASP	3.7
1	C	276	ALA	3.6
1	F	280	LEU	3.5
1	C	151	ALA	3.5
1	F	275	VAL	3.5
1	C	278	ASN	3.3
1	C	279	GLU	3.2
1	E	269	TYR	3.1
1	B	39	ILE	3.1
1	B	55	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	277	MET	3.0
1	A	278	ASN	3.0
1	C	148	THR	3.0
1	E	142	LYS	2.9
1	F	279	GLU	2.9
1	A	280	LEU	2.9
1	E	88	ALA	2.8
1	F	276	ALA	2.8
1	E	99	ALA	2.8
1	B	119	SER	2.7
1	C	115	VAL	2.7
1	E	166	TYR	2.7
1	B	54	VAL	2.7
1	E	199	THR	2.7
1	C	146	PHE	2.6
1	F	195	MET	2.6
1	F	173	GLN	2.5
1	E	278	ASN	2.5
1	A	164	THR	2.5
1	C	147	ALA	2.5
1	C	62	GLU	2.4
1	F	123	ASP	2.4
1	C	128	PHE	2.4
1	C	234	LEU	2.3
1	B	94	ASP	2.3
1	E	120	GLU	2.3
1	F	202	ARG	2.3
1	B	63	ILE	2.3
1	D	265	GLU	2.2
1	B	275	VAL	2.2
1	E	105	GLY	2.2
1	B	154	MET	2.2
1	C	61	LEU	2.1
1	B	80	LEU	2.1
1	F	88	ALA	2.1
1	E	268	THR	2.1
1	F	65	LEU	2.1
1	B	91	ILE	2.1
1	C	99	ALA	2.1
1	C	105	GLY	2.1
1	F	85	ILE	2.0
1	B	118	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	100	MET	2.0
1	C	65	LEU	2.0
1	C	108	ILE	2.0
1	C	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 [\(i\)](#)

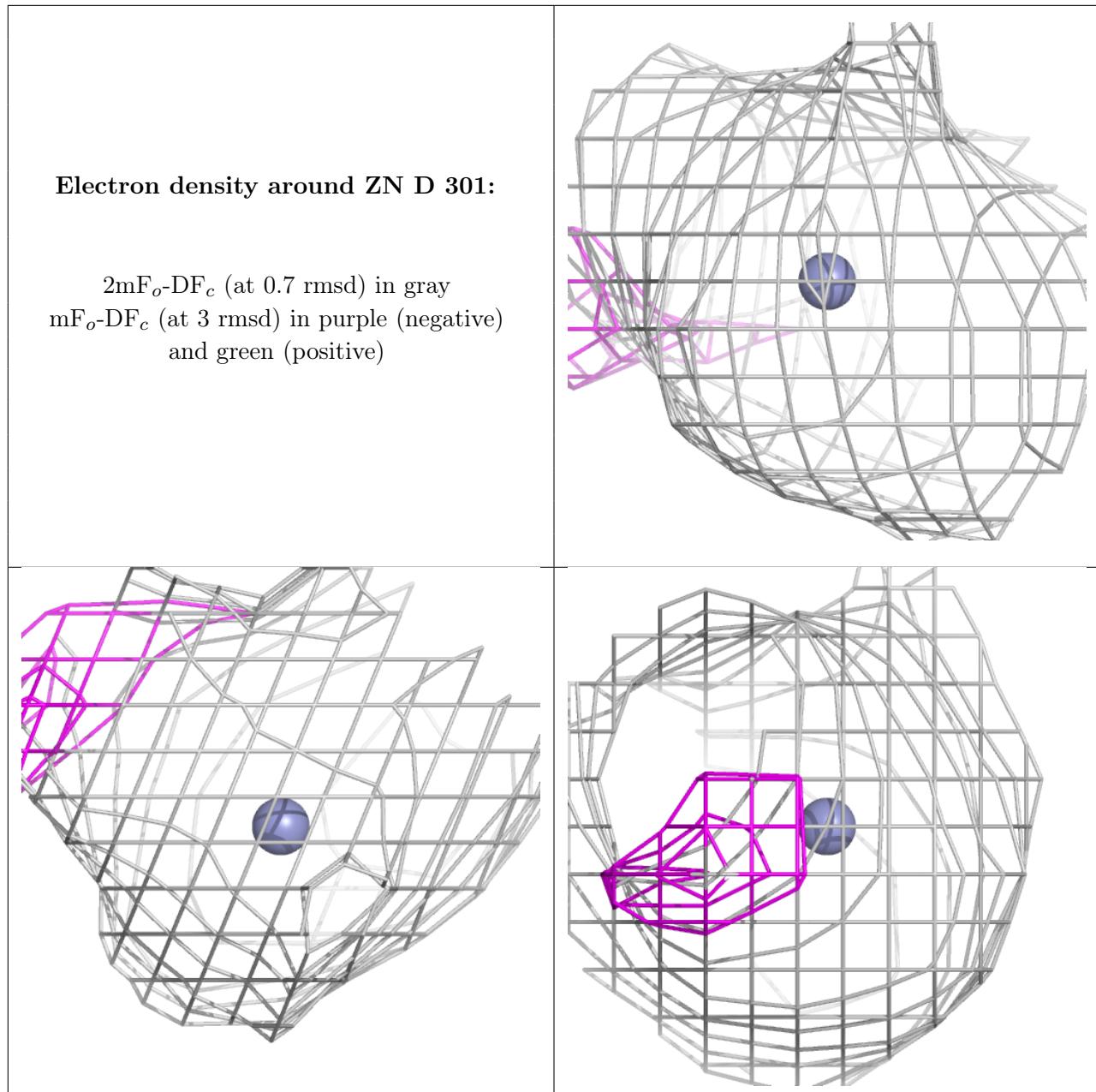
There are no monosaccharides in this entry.

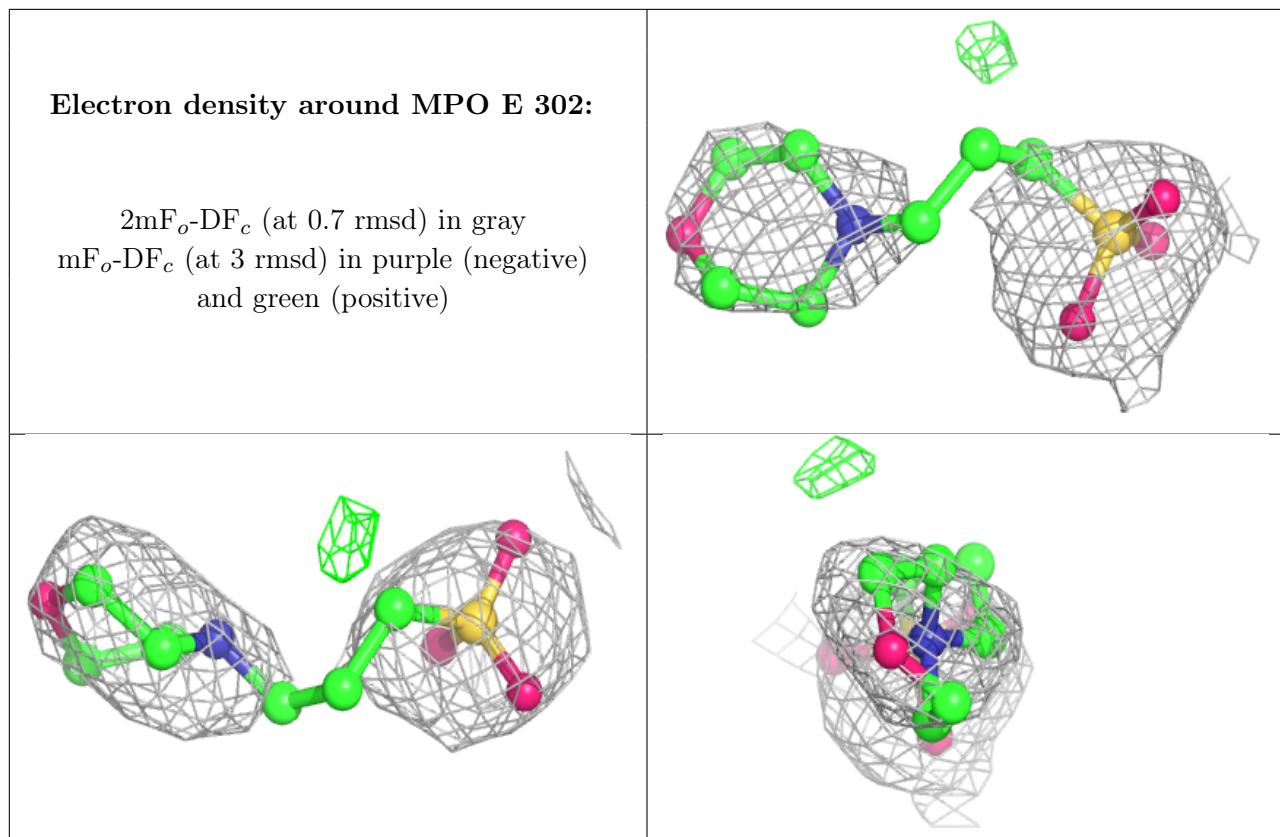
## 6.4 Ligands [\(i\)](#)

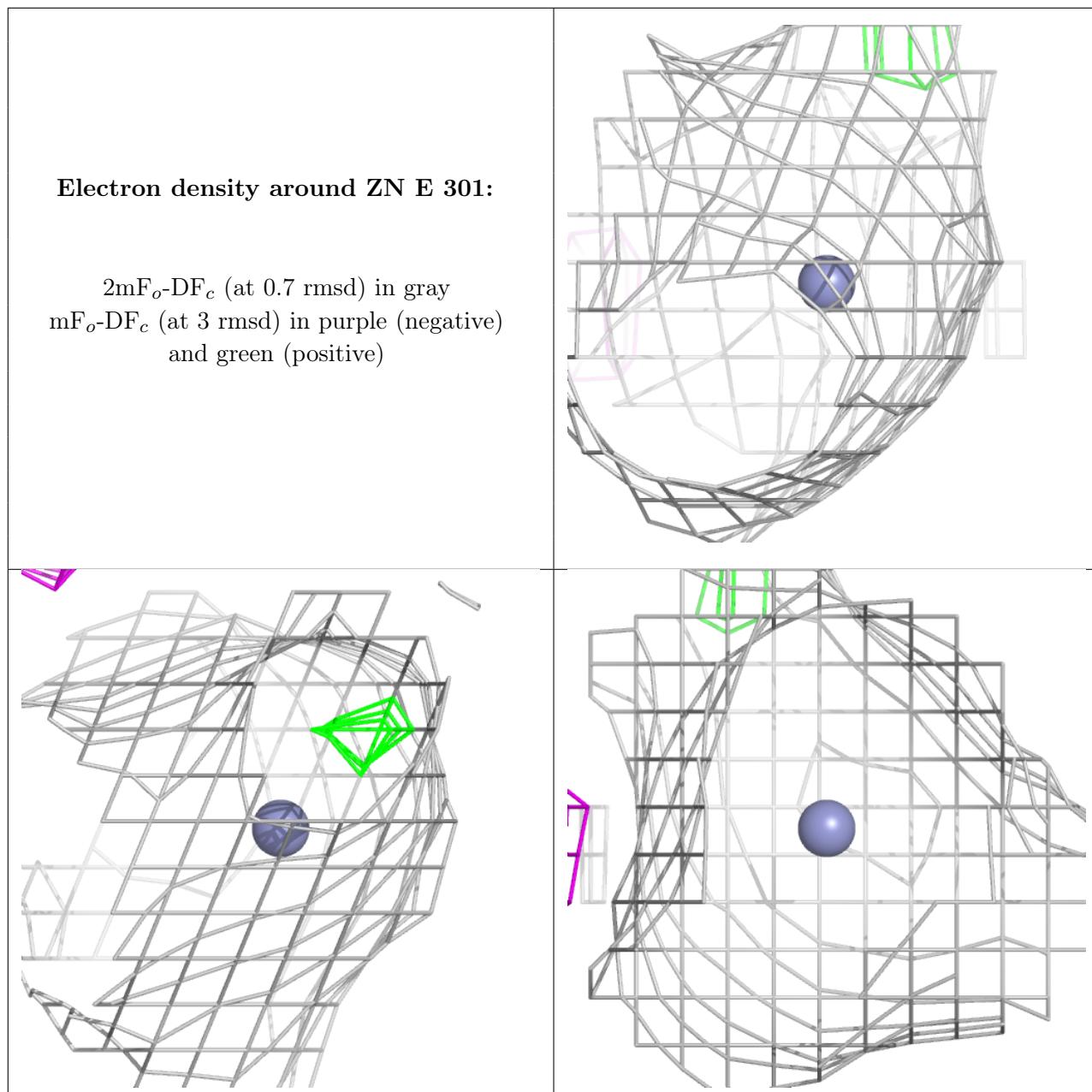
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

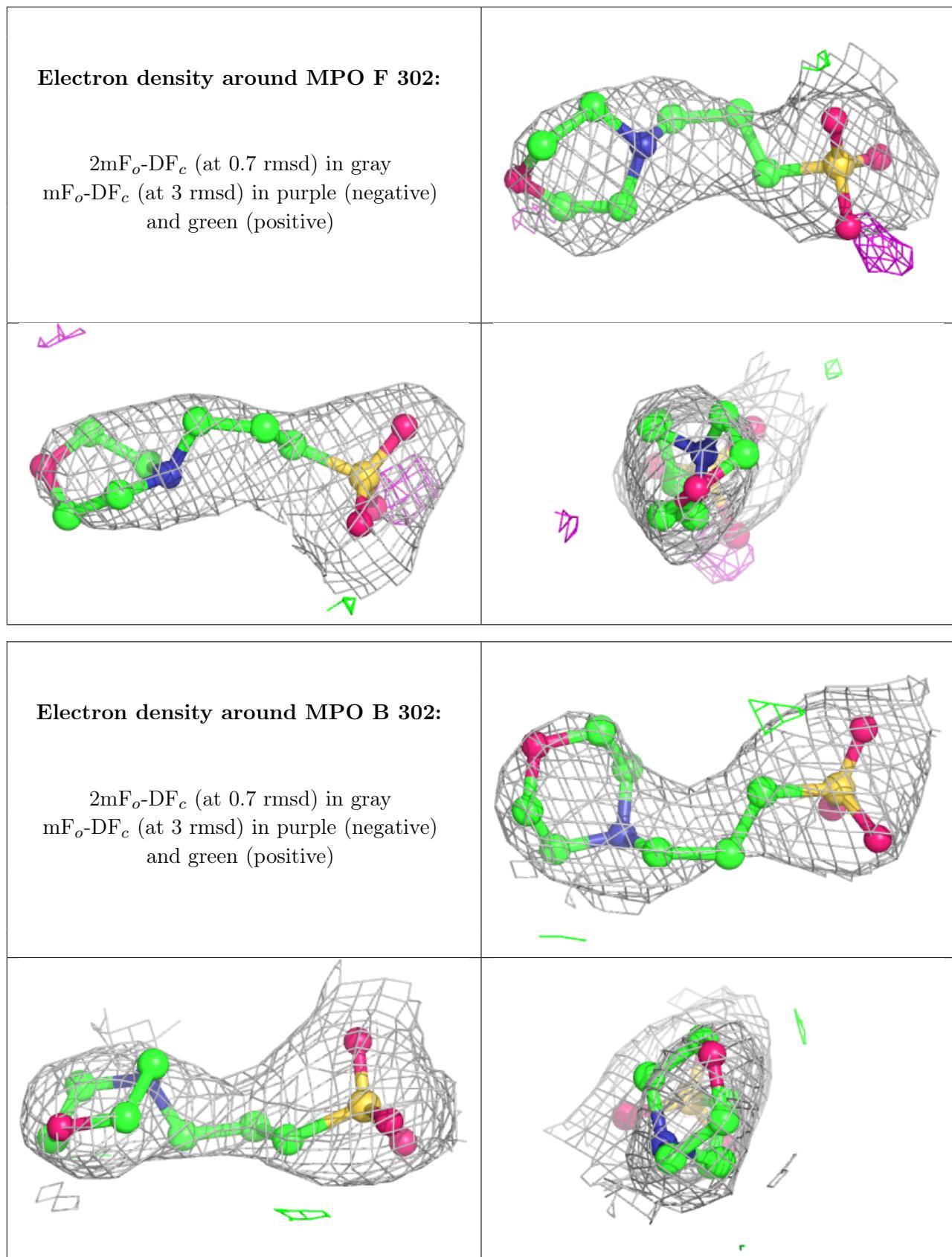
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	D	301	1/1	0.88	0.06	163,163,163,163	0
3	MPO	E	302	13/13	0.89	0.29	102,114,124,128	0
2	ZN	E	301	1/1	0.92	0.12	134,134,134,134	0
3	MPO	F	302	13/13	0.93	0.23	93,102,108,117	0
3	MPO	B	302	13/13	0.94	0.18	80,92,114,116	0
3	MPO	A	302	13/13	0.95	0.19	86,96,102,102	0
2	ZN	C	301	1/1	0.98	0.04	122,122,122,122	0
2	ZN	A	301	1/1	0.98	0.12	87,87,87,87	0
2	ZN	B	301	1/1	0.98	0.07	108,108,108,108	0
2	ZN	F	301	1/1	0.98	0.07	110,110,110,110	0

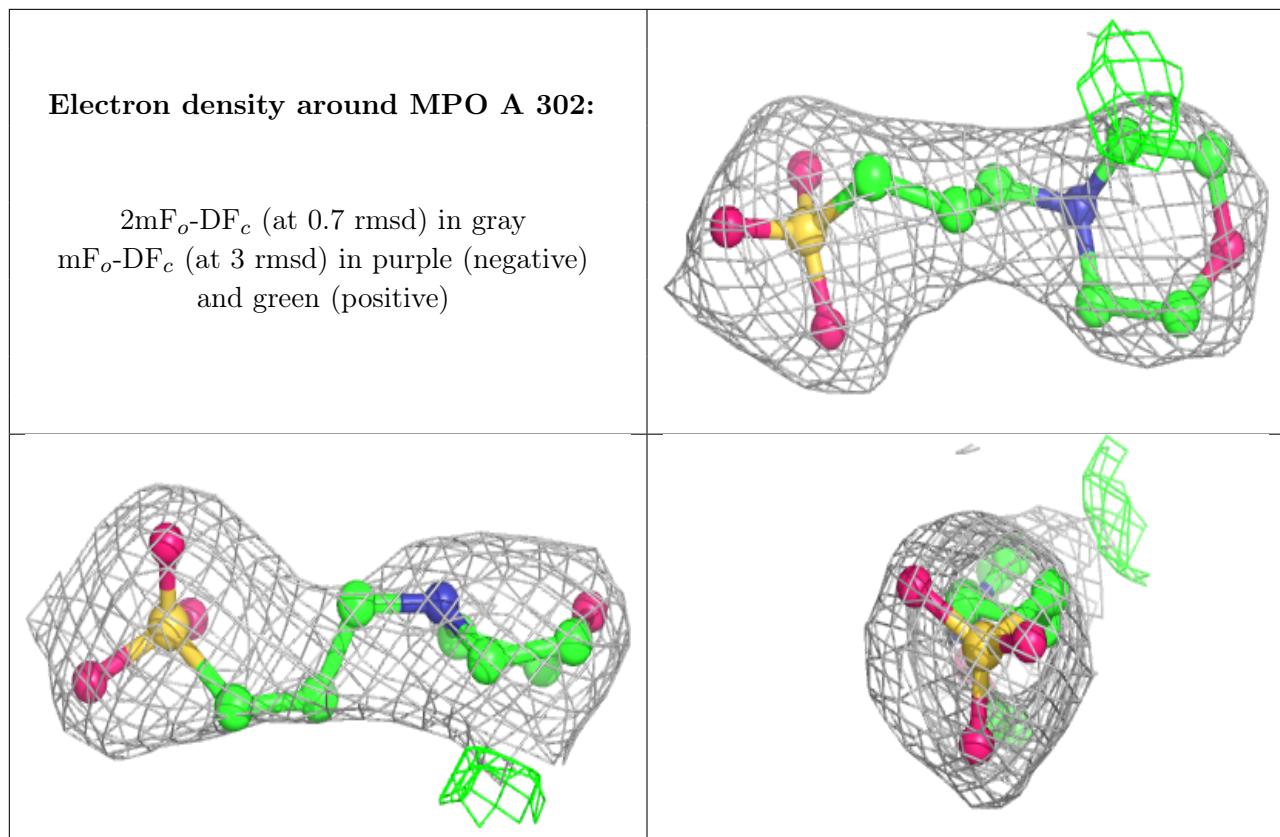
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

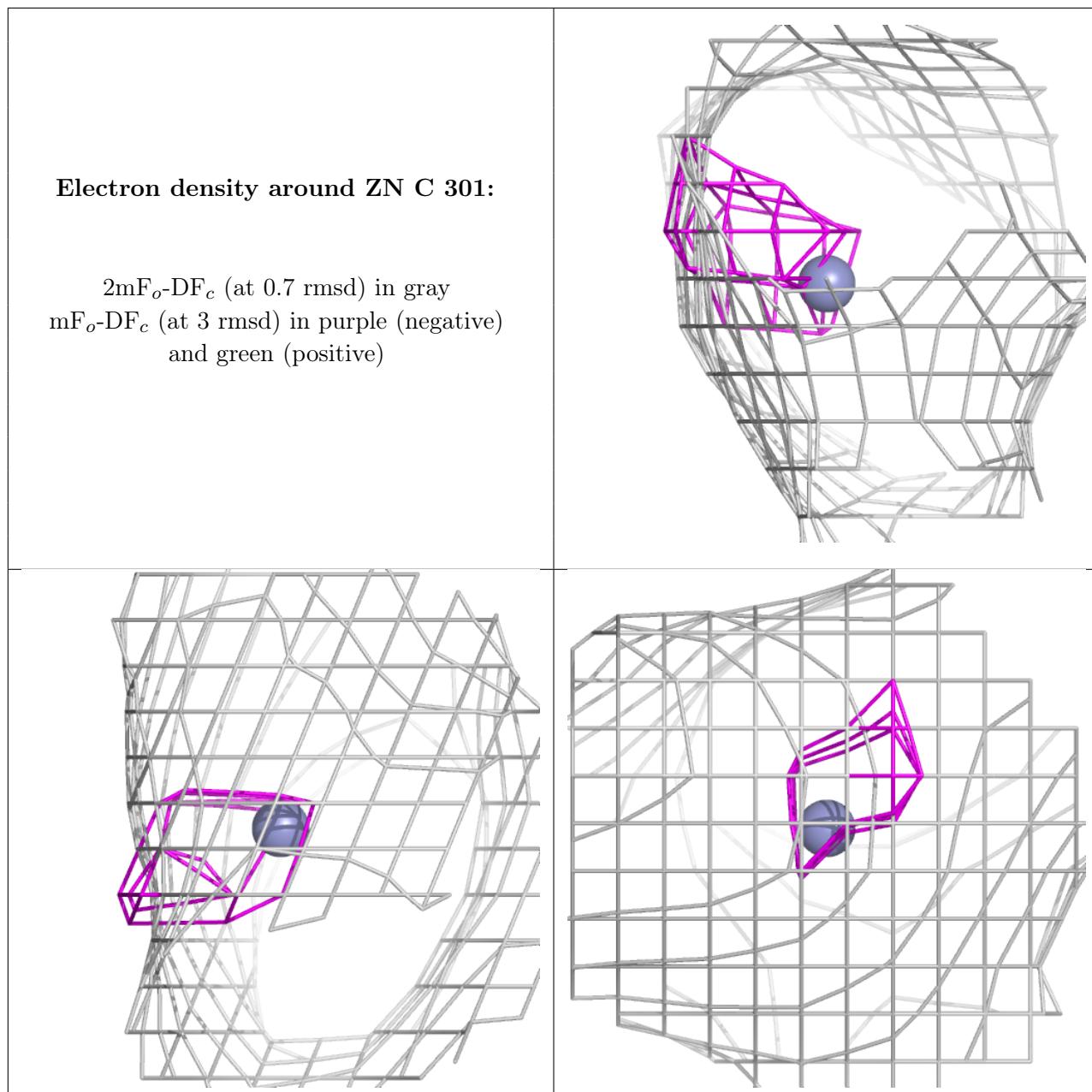


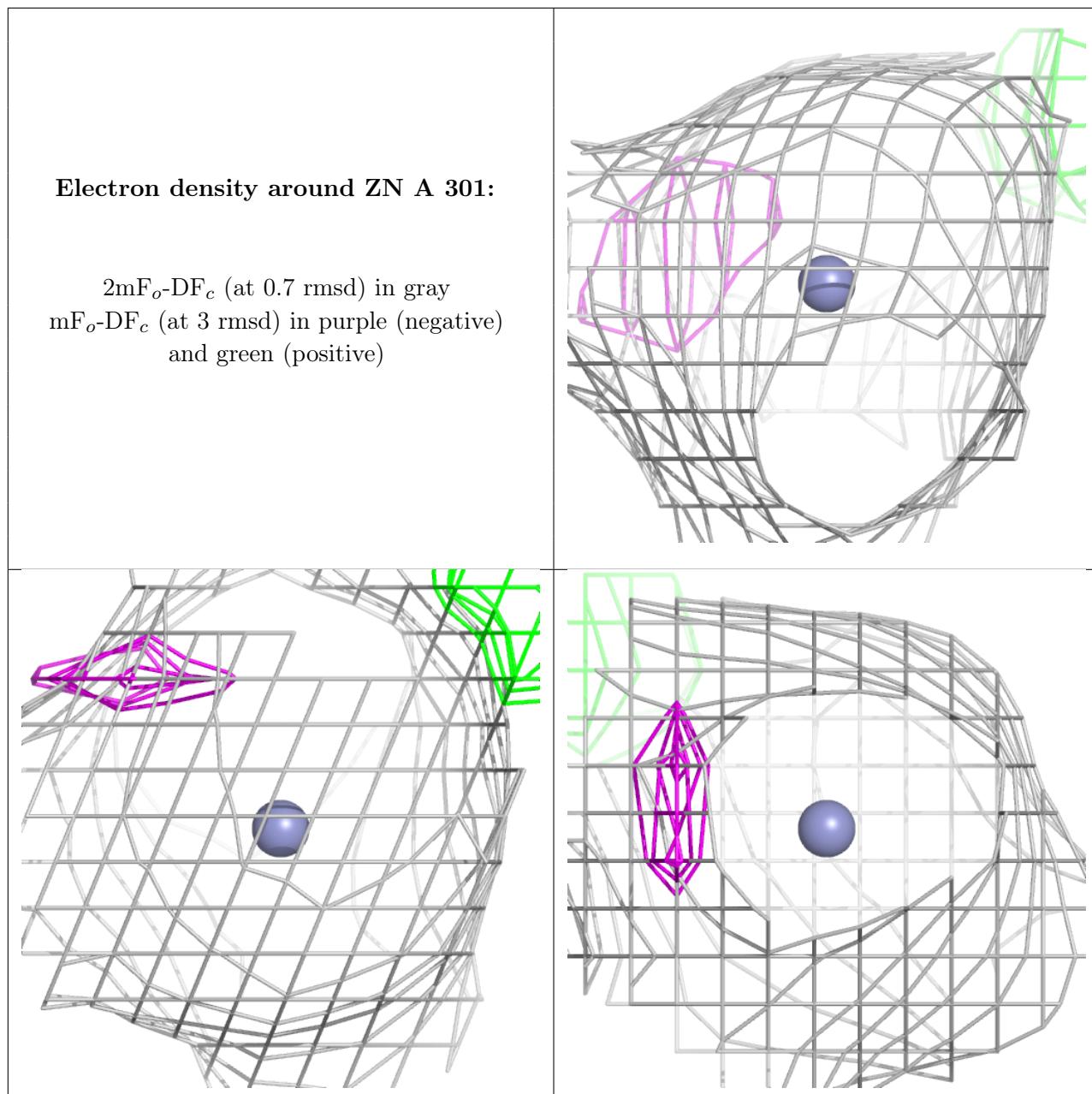


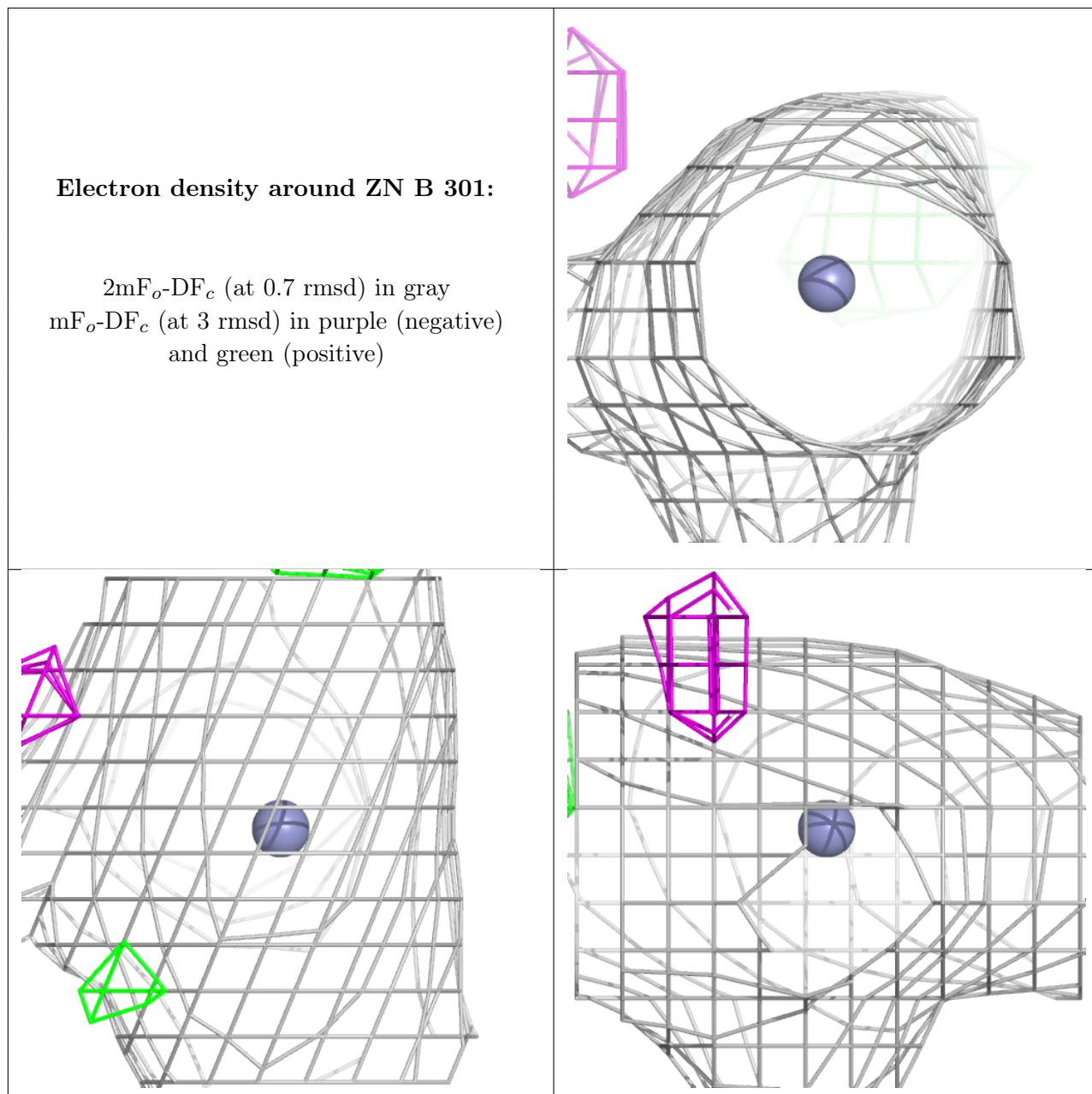


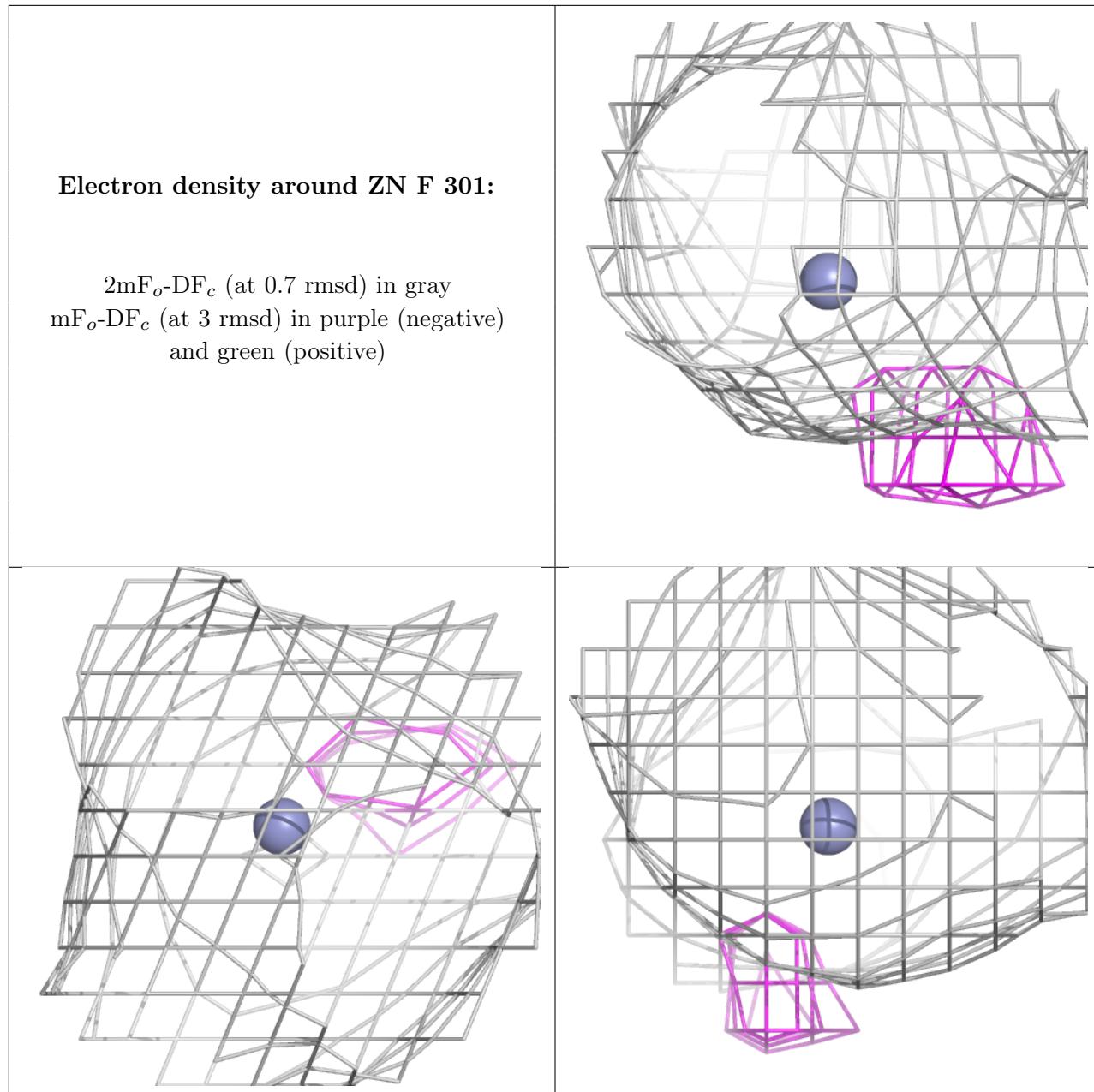












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.