



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2022 – 06:25 PM JST

PDB ID : 7EEU
Title : Human p53 core domain with hot spot mutation R282W in complex with the natural CDKN1A(p21) p53-response element and Arsenic
Authors : Xing, Y.F.; Lu, M.
Deposited on : 2021-03-19
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

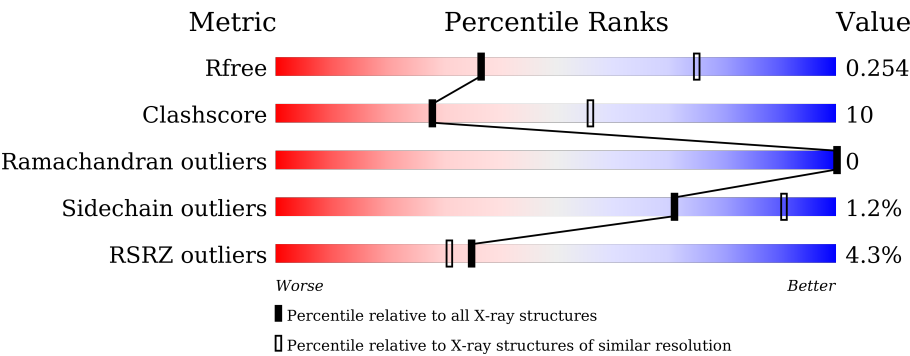
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







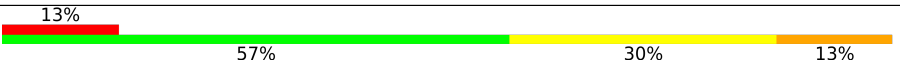
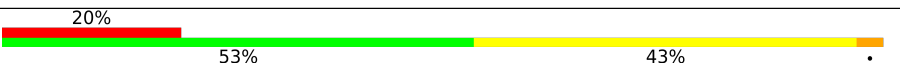
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	200	<div><div>2%</div><div>83%</div><div>16%</div><div>.</div></div>
1	B	200	<div><div>2%</div><div>81%</div><div>18%</div><div>.</div></div>
1	C	200	<div><div>6%</div><div>81%</div><div>17%</div><div>..</div></div>
1	D	200	<div><div>6%</div><div>80%</div><div>18%</div><div>.</div></div>
1	E	200	<div><div>%</div><div>79%</div><div>18%</div><div>..</div></div>
1	F	200	<div><div>2%</div><div>82%</div><div>16%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	G	200	
1	H	200	
2	I	30	
2	K	30	
3	J	30	
3	L	30	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14988 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1561	965	288	292	16			
1	B	198	Total	C	N	O	S	0	0	0
			1561	965	288	292	16			
1	C	198	Total	C	N	O	S	0	0	0
			1561	965	288	292	16			
1	D	198	Total	C	N	O	S	0	0	0
			1561	965	288	292	16			
1	E	198	Total	C	N	O	S	0	0	0
			1561	965	288	292	16			
1	F	197	Total	C	N	O	S	0	0	0
			1555	962	287	290	16			
1	G	198	Total	C	N	O	S	0	0	0
			1561	965	288	292	16			
1	H	198	Total	C	N	O	S	0	0	0
			1561	965	288	292	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	TRP	ARG	engineered mutation	UNP P04637
B	282	TRP	ARG	engineered mutation	UNP P04637
C	282	TRP	ARG	engineered mutation	UNP P04637
D	282	TRP	ARG	engineered mutation	UNP P04637
E	282	TRP	ARG	engineered mutation	UNP P04637
F	282	TRP	ARG	engineered mutation	UNP P04637
G	282	TRP	ARG	engineered mutation	UNP P04637
H	282	TRP	ARG	engineered mutation	UNP P04637

- Molecule 2 is a DNA chain called CDKN1A(p21) sense strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	30	Total	C	N	O	P	0	0	0
			616	292	116	178	30			
2	K	30	Total	C	N	O	P	0	0	0
			616	292	116	178	30			

- Molecule 3 is a DNA chain called CDKN1A(p21) anti-sense strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	30	Total	C	N	O	P	0	0	0
			614	292	110	182	30			
3	L	30	Total	C	N	O	P	0	0	0
			614	292	110	182	30			

- Molecule 4 is ARSENIC (three-letter code: ARS) (formula: As) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	As	0	0
			1	1		
4	B	1	Total	As	0	0
			1	1		
4	C	1	Total	As	0	0
			1	1		
4	D	1	Total	As	0	0
			1	1		
4	E	1	Total	As	0	0
			1	1		
4	F	1	Total	As	0	0
			1	1		
4	G	1	Total	As	0	0
			1	1		
4	H	1	Total	As	0	0
			1	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

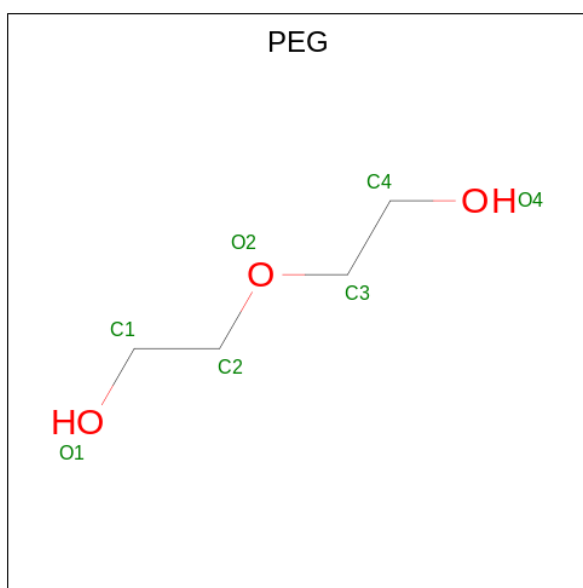
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		
5	G	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	B	2	Total	O	0	0
			2	2		

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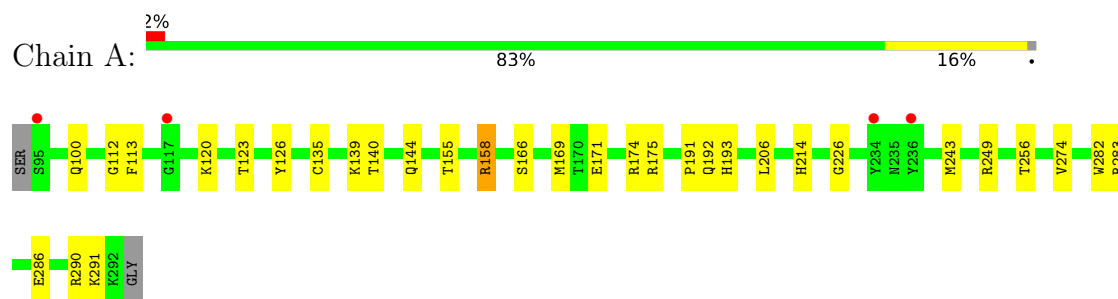
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total 2	O 2	0	0
7	D	2	Total 2	O 2	0	0
7	E	2	Total 2	O 2	0	0
7	F	1	Total 1	O 1	0	0
7	G	2	Total 2	O 2	0	0
7	H	1	Total 1	O 1	0	0
7	K	1	Total 1	O 1	0	0

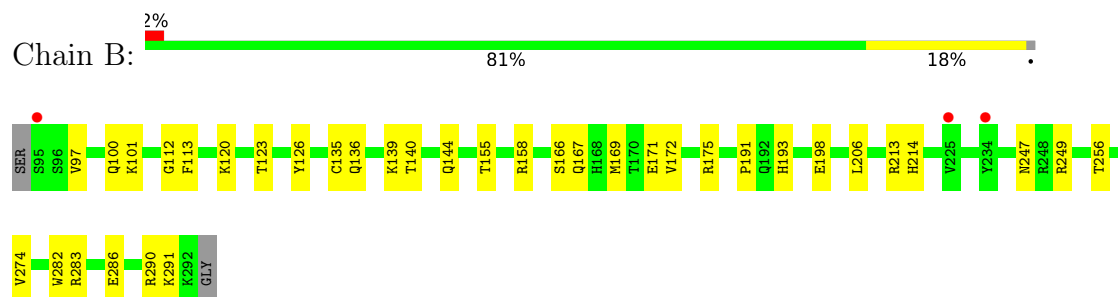
3 Residue-property plots [i](#)

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.

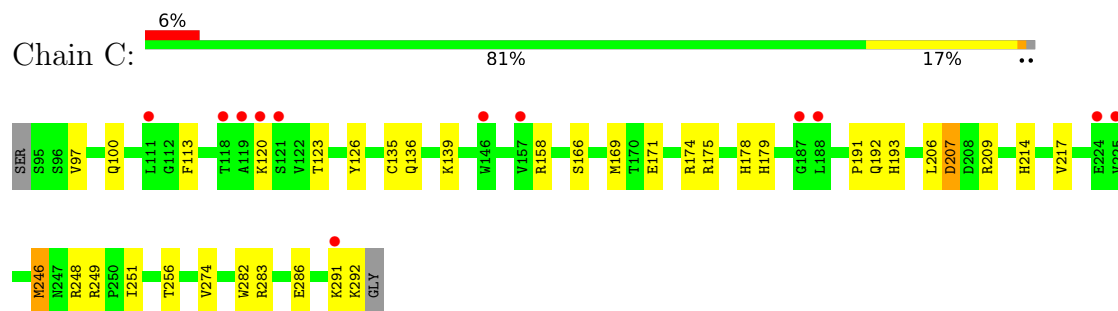
- Molecule 1: Cellular tumor antigen p53



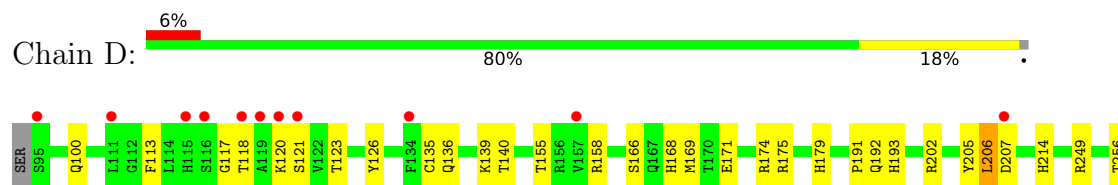
- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53

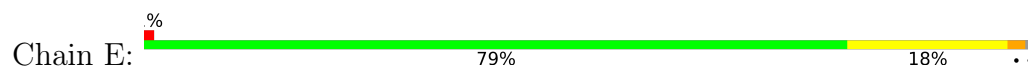


- Molecule 1: Cellular tumor antigen p53

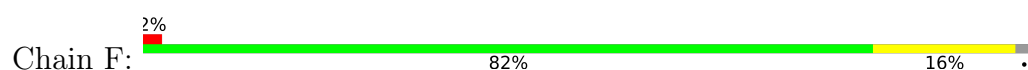




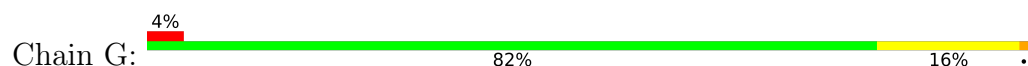
- Molecule 1: Cellular tumor antigen p53



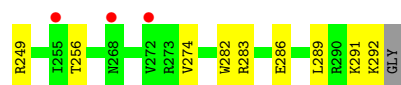
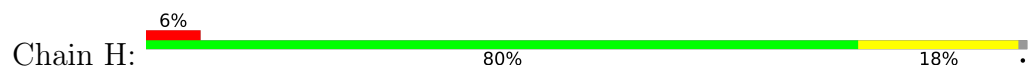
- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



- Molecule 2: CDKN1A(p21) sense strand

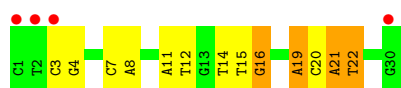




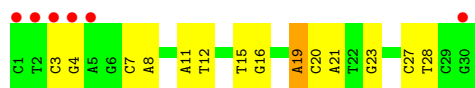
- Molecule 2: CDKN1A(p21) sense strand



- Molecule 3: CDKN1A(p21) anti-sense strand



- Molecule 3: CDKN1A(p21) anti-sense strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.81Å 95.58Å 99.65Å 89.62° 89.85° 75.79°	Depositor
Resolution (Å)	45.39 – 2.90 45.38 – 2.88	Depositor EDS
% Data completeness (in resolution range)	84.8 (45.39-2.90) 95.7 (45.38-2.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.234 , 0.264 0.229 , 0.254	Depositor DCC
R_{free} test set	2948 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.115 for -h,-k,l	Xtriage
Reported twinning fraction	0.739 for H, K, L 0.261 for -h,-k,l	Depositor
Outliers	0 of 57040 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14988	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9013e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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, ARS, PEG

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	0.64	0/1598	0.75	1/2166 (0.0%)
1	B	0.60	0/1598	0.75	0/2166
1	C	0.60	0/1598	0.78	3/2166 (0.1%)
1	D	0.61	0/1598	0.81	5/2166 (0.2%)
1	E	0.61	0/1598	0.78	5/2166 (0.2%)
1	F	0.60	0/1592	0.75	1/2158 (0.0%)
1	G	0.60	0/1598	0.80	2/2166 (0.1%)
1	H	0.58	0/1598	0.77	0/2166
2	I	0.80	1/691 (0.1%)	0.95	0/1064
2	K	0.62	0/691	0.90	0/1064
3	J	0.84	1/687 (0.1%)	1.08	5/1058 (0.5%)
3	L	0.66	0/687	0.97	1/1058 (0.1%)
All	All	0.63	2/15534 (0.0%)	0.82	23/21564 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	9	DA	O3'-P	-5.70	1.54	1.61
3	J	14	DT	C2'-C1'	5.25	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	22	DT	O5'-P-OP2	8.86	121.34	110.70
1	E	248	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	G	174	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	D	202	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	E	158	ARG	NE-CZ-NH1	-6.65	116.98	120.30
1	A	158	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	D	207	ASP	CB-CG-OD2	-6.41	112.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	22	DT	O5'-P-OP1	-6.01	100.29	105.70
1	D	207	ASP	CB-CG-OD1	5.97	123.68	118.30
3	J	16	DG	O5'-P-OP1	-5.96	100.33	105.70
1	C	207	ASP	CB-CG-OD1	5.96	123.67	118.30
3	J	21	DA	O5'-P-OP1	-5.90	100.39	105.70
1	C	207	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	C	246	MET	CG-SD-CE	5.83	109.53	100.20
1	E	249	ARG	CG-CD-NE	5.79	123.97	111.80
1	E	248	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	D	202	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	207	ASP	CB-CG-OD2	-5.54	113.31	118.30
3	J	19	DA	O5'-P-OP1	-5.48	100.77	105.70
1	E	174	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	D	206	LEU	CB-CG-CD1	5.32	120.04	111.00
3	L	19	DA	O5'-P-OP1	-5.27	100.96	105.70
1	F	248	ARG	NE-CZ-NH1	-5.13	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1561	0	1518	27	0
1	B	1561	0	1518	26	0
1	C	1561	0	1518	37	0
1	D	1561	0	1518	25	0
1	E	1561	0	1518	26	0
1	F	1555	0	1513	28	0
1	G	1561	0	1518	43	0
1	H	1561	0	1518	34	0
2	I	616	0	337	16	0
2	K	616	0	337	14	0
3	J	614	0	339	23	0
3	L	614	0	339	13	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	E	7	0	10	1	0
6	F	7	0	10	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	G	2	0	0	0	0
7	H	1	0	0	0	0
7	K	1	0	0	0	0
All	All	14988	0	13511	263	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 10.

All (263) 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:H:121:SER:HB3	2:K:15:DC:OP2	1.42	1.18
1:E:227:SER:HB2	1:F:101:LYS:NZ	1.66	1.11
1:E:227:SER:HB2	1:F:101:LYS:HZ2	1.11	1.07
1:F:174:ARG:HD3	1:F:192:GLN:OE1	1.58	1.04
2:I:10:DT:N3	3:J:21:DA:N1	2.08	0.99
2:I:19:DA:N1	3:J:12:DT:N3	2.14	0.95
1:A:123:THR:HG22	1:A:139:LYS:HG2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:20:DT:N3	3:J:11:DA:N1	2.16	0.93
2:I:9:DA:N1	3:J:22:DT:N3	2.16	0.92
1:F:120:LYS:HD2	3:L:7:DC:H5'	1.53	0.89
1:E:177:PRO:HD2	1:E:244:GLY:HA3	1.54	0.87
1:A:123:THR:CG2	1:A:139:LYS:HG2	2.06	0.86
1:E:227:SER:CB	1:F:101:LYS:NZ	2.40	0.84
1:A:123:THR:HG21	1:A:139:LYS:HD3	1.61	0.82
1:B:247:ASN:O	1:B:247:ASN:ND2	2.13	0.81
1:H:175:ARG:HG3	1:H:238:CYS:SG	2.20	0.80
2:I:20:DT:O4	3:J:11:DA:N6	2.15	0.80
1:H:175:ARG:HE	1:H:179:HIS:HB3	1.46	0.79
1:C:246:MET:HE3	1:C:251:ILE:HG23	1.65	0.78
1:E:158:ARG:HH22	1:E:206:LEU:HD23	1.49	0.77
1:A:158:ARG:HH22	1:A:206:LEU:HD23	1.50	0.76
1:A:140:THR:HG21	1:B:166:SER:HB2	1.67	0.76
1:G:166:SER:OG	1:H:140:THR:HG21	1.86	0.76
1:H:175:ARG:NE	1:H:179:HIS:HB3	2.00	0.75
1:G:96:SER:HB3	1:G:211:THR:HG22	1.70	0.74
1:A:123:THR:HG21	1:A:139:LYS:CD	2.20	0.70
3:J:15:DT:H2''	3:J:16:DG:C8	2.26	0.70
1:C:246:MET:HE1	1:C:251:ILE:HG12	1.72	0.69
1:B:120:LYS:HD2	3:J:7:DC:C5'	2.22	0.69
1:G:174:ARG:NH1	1:G:192:GLN:CD	2.48	0.68
1:F:120:LYS:HD2	3:L:7:DC:C5'	2.24	0.67
1:B:171:GLU:OE1	1:B:249:ARG:NH2	2.24	0.67
1:F:283:ARG:O	1:F:287:GLU:HG2	1.95	0.67
3:L:15:DT:H2''	3:L:16:DG:C8	2.29	0.66
1:C:209:ARG:HB2	1:G:174:ARG:NH2	2.09	0.66
1:H:174:ARG:NH2	1:H:192:GLN:HB3	2.12	0.65
1:H:282:TRP:HE3	1:H:283:ARG:HG3	1.60	0.65
1:C:246:MET:CE	1:C:251:ILE:HG23	2.26	0.65
1:E:243:MET:O	1:E:243:MET:HG2	1.96	0.65
1:A:123:THR:CG2	1:A:139:LYS:CG	2.75	0.64
1:B:158:ARG:HH12	1:B:206:LEU:HD23	1.63	0.64
1:G:158:ARG:HH12	1:G:206:LEU:HD23	1.64	0.63
1:D:282:TRP:CZ2	1:D:286:GLU:OE1	2.51	0.62
1:F:158:ARG:HH12	1:F:206:LEU:HD23	1.63	0.62
1:E:227:SER:CB	1:F:101:LYS:HZ2	1.99	0.61
1:F:193:HIS:CE1	1:F:214:HIS:HB3	2.36	0.61
1:D:121:SER:HB3	2:I:15:DC:OP2	2.01	0.60
1:B:120:LYS:HD2	3:J:7:DC:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLN:NE2	1:G:206:LEU:HD11	2.16	0.60
1:G:174:ARG:HH11	1:G:192:GLN:HB3	1.67	0.60
1:G:174:ARG:HH11	1:G:192:GLN:CG	2.14	0.60
1:A:139:LYS:HD2	1:B:167:GLN:OE1	2.02	0.59
1:A:174:ARG:HD3	1:A:192:GLN:NE2	2.17	0.59
1:H:175:ARG:CZ	1:H:237:MET:HB3	2.32	0.59
1:D:205:TYR:C	1:D:206:LEU:HD22	2.24	0.58
3:J:11:DA:H2''	3:J:12:DT:H5'	1.85	0.58
1:E:193:HIS:CE1	1:E:214:HIS:HB3	2.39	0.58
1:A:174:ARG:HD3	1:A:192:GLN:HE21	1.68	0.58
1:B:290:ARG:NH1	1:B:291:LYS:HE2	2.19	0.58
1:G:95:SER:O	1:H:201:LEU:HD13	2.04	0.57
1:A:139:LYS:HE3	1:A:140:THR:O	2.04	0.57
1:B:193:HIS:CE1	1:B:214:HIS:HB3	2.39	0.57
1:C:206:LEU:HD12	1:C:217:VAL:HG23	1.87	0.57
3:L:19:DA:H2''	3:L:20:DC:H5''	1.86	0.56
1:C:214:HIS:HE1	1:G:207:ASP:OD2	1.88	0.56
1:H:113:PHE:CD1	1:H:126:TYR:CE2	2.93	0.56
1:A:193:HIS:CE1	1:A:214:HIS:HB3	2.40	0.56
2:I:29:DA:H2''	2:I:30:DG:C8	2.41	0.56
3:J:19:DA:H2''	3:J:20:DC:H5''	1.88	0.56
1:C:192:GLN:OE1	1:G:207:ASP:O	2.24	0.56
1:G:175:ARG:HD3	1:G:191:PRO:O	2.06	0.56
1:D:136:GLN:HB3	1:D:139:LYS:CG	2.37	0.55
1:E:242:CYS:O	1:E:247:ASN:HA	2.05	0.55
1:H:193:HIS:CE1	1:H:214:HIS:HB3	2.41	0.55
1:C:246:MET:CE	1:C:251:ILE:CG2	2.84	0.55
1:G:97:VAL:HG12	1:G:97:VAL:O	2.07	0.55
3:L:15:DT:H2''	3:L:16:DG:N7	2.21	0.55
1:D:193:HIS:CE1	1:D:214:HIS:HB3	2.43	0.54
1:E:140:THR:HG21	1:F:166:SER:HB2	1.89	0.54
2:I:7:DA:C2	2:I:8:DC:C2	2.95	0.54
2:I:19:DA:H2	3:J:12:DT:O2	1.90	0.54
1:C:193:HIS:CE1	1:C:214:HIS:HB3	2.43	0.54
1:H:136:GLN:HB3	1:H:139:LYS:CG	2.36	0.54
1:H:114:LEU:HD23	1:H:142:PRO:HG2	1.90	0.54
2:K:29:DA:H2''	2:K:30:DG:C8	2.42	0.54
1:C:136:GLN:HB3	1:C:139:LYS:CG	2.38	0.54
1:G:136:GLN:HB3	1:G:139:LYS:CG	2.37	0.54
1:F:171:GLU:OE1	1:F:249:ARG:NH1	2.39	0.54
1:G:282:TRP:CE2	1:G:286:GLU:OE1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:GLN:HB3	1:F:139:LYS:CG	2.39	0.53
1:G:193:HIS:CE1	1:G:214:HIS:HB3	2.43	0.53
1:A:166:SER:HA	1:A:169:MET:HG3	1.90	0.53
1:H:171:GLU:OE1	1:H:249:ARG:NH1	2.37	0.53
2:I:20:DT:C4	3:J:11:DA:N1	2.76	0.53
3:L:11:DA:H2''	3:L:12:DT:H5'	1.91	0.53
1:D:166:SER:HA	1:D:169:MET:HG3	1.91	0.53
1:G:166:SER:HA	1:G:169:MET:HG3	1.91	0.53
1:C:282:TRP:CE2	1:C:286:GLU:OE1	2.62	0.53
1:G:175:ARG:HH21	1:G:179:HIS:HB3	1.73	0.53
1:E:136:GLN:HB3	1:E:139:LYS:CG	2.39	0.52
1:G:175:ARG:NH2	1:G:179:HIS:HB3	2.23	0.52
1:B:136:GLN:HB3	1:B:139:LYS:CG	2.39	0.52
1:H:166:SER:HA	1:H:169:MET:HG3	1.92	0.52
1:A:243:MET:HE2	1:C:178:HIS:HD2	1.75	0.52
1:C:166:SER:HA	1:C:169:MET:HG3	1.92	0.52
1:C:206:LEU:HD12	1:C:217:VAL:CG2	2.39	0.52
3:L:3:DC:H4'	3:L:4:DG:OP1	2.10	0.52
1:D:175:ARG:HD3	1:D:191:PRO:O	2.10	0.52
1:E:166:SER:HA	1:E:169:MET:HG3	1.92	0.52
2:K:7:DA:C2	2:K:8:DC:C2	2.97	0.52
3:J:3:DC:H4'	3:J:4:DG:OP1	2.10	0.51
1:A:120:LYS:HA	1:A:283:ARG:NH1	2.26	0.51
1:E:120:LYS:HA	1:E:283:ARG:NH1	2.26	0.51
1:G:120:LYS:HA	1:G:283:ARG:NH1	2.26	0.51
1:G:174:ARG:HH11	1:G:192:GLN:CB	2.23	0.51
1:D:120:LYS:HA	1:D:283:ARG:NH1	2.26	0.51
1:C:120:LYS:HA	1:C:283:ARG:NH1	2.26	0.51
1:E:177:PRO:HD2	1:E:244:GLY:CA	2.34	0.51
1:B:97:VAL:HG11	1:B:169:MET:HG3	1.93	0.50
1:D:123:THR:HG23	1:D:139:LYS:HG3	1.94	0.50
1:B:120:LYS:HA	1:B:283:ARG:NH1	2.27	0.50
1:A:140:THR:HG21	1:B:166:SER:CB	2.38	0.50
1:D:206:LEU:HD22	1:D:206:LEU:N	2.26	0.50
1:B:120:LYS:HB2	3:J:7:DC:OP1	2.12	0.50
1:C:123:THR:HG23	1:C:139:LYS:HG3	1.94	0.49
1:F:174:ARG:CD	1:F:192:GLN:OE1	2.45	0.49
1:D:192:GLN:OE1	1:H:207:ASP:O	2.30	0.49
1:H:291:LYS:O	1:H:292:LYS:C	2.50	0.49
3:J:15:DT:H2''	3:J:16:DG:N7	2.26	0.49
1:F:120:LYS:HA	1:F:283:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:DG:H2''	2:I:12:DT:H5''	1.95	0.49
1:H:174:ARG:HH22	1:H:192:GLN:CD	2.16	0.49
1:B:123:THR:HG23	1:B:139:LYS:HG3	1.95	0.49
2:K:11:DG:H2''	2:K:12:DT:H5''	1.95	0.49
2:I:19:DA:C2	3:J:12:DT:O2	2.65	0.49
1:H:121:SER:CB	2:K:15:DC:OP2	2.36	0.49
1:D:206:LEU:HD12	1:H:192:GLN:NE2	2.28	0.48
1:H:113:PHE:CD1	1:H:126:TYR:CD2	3.02	0.48
1:E:158:ARG:HG2	1:E:256:THR:OG1	2.14	0.48
1:G:123:THR:HG23	1:G:139:LYS:HG3	1.96	0.48
1:G:291:LYS:HG3	1:G:292:LYS:H	1.79	0.48
1:H:123:THR:HG23	1:H:139:LYS:HG3	1.95	0.48
2:I:20:DT:H1'	2:I:21:DG:C8	2.48	0.48
1:E:123:THR:HG23	1:E:139:LYS:HG3	1.96	0.48
1:C:97:VAL:HG13	1:C:97:VAL:O	2.12	0.48
1:D:136:GLN:HB3	1:D:139:LYS:HG3	1.95	0.48
1:B:172:VAL:HG22	1:B:213:ARG:HD3	1.95	0.48
1:C:171:GLU:OE1	1:C:249:ARG:NH1	2.40	0.48
1:F:158:ARG:HG2	1:F:256:THR:OG1	2.14	0.48
1:H:136:GLN:HB3	1:H:139:LYS:HG3	1.94	0.48
1:G:120:LYS:HB2	2:K:5:DG:P	2.54	0.48
1:B:282:TRP:CE2	1:B:286:GLU:OE1	2.67	0.47
1:H:114:LEU:HD22	1:H:114:LEU:N	2.29	0.47
1:F:282:TRP:CE2	1:F:286:GLU:OE1	2.67	0.47
1:C:174:ARG:NH2	1:G:207:ASP:O	2.47	0.47
1:G:120:LYS:HB2	2:K:5:DG:OP2	2.15	0.47
1:D:158:ARG:HG2	1:D:256:THR:OG1	2.14	0.47
1:F:243:MET:CG	1:H:178:HIS:CD2	2.97	0.47
1:G:136:GLN:HB3	1:G:139:LYS:HG3	1.95	0.47
1:G:158:ARG:HG2	1:G:256:THR:OG1	2.15	0.47
1:H:175:ARG:CG	1:H:238:CYS:SG	2.98	0.47
1:C:136:GLN:HB3	1:C:139:LYS:HG3	1.97	0.47
1:C:158:ARG:HG2	1:C:256:THR:OG1	2.14	0.47
1:F:123:THR:HG23	1:F:139:LYS:HG3	1.96	0.47
1:G:174:ARG:HH12	1:G:192:GLN:NE2	2.13	0.47
1:H:158:ARG:HG2	1:H:256:THR:OG1	2.15	0.47
2:K:20:DT:H1'	2:K:21:DG:C8	2.50	0.47
1:C:291:LYS:HG3	1:C:292:LYS:H	1.80	0.47
1:A:158:ARG:HG2	1:A:256:THR:OG1	2.14	0.46
1:G:96:SER:O	1:G:98:PRO:HD3	2.16	0.46
1:G:140:THR:HG1	1:G:198:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLN:HB3	1:B:139:LYS:HG3	1.96	0.46
1:F:140:THR:HG1	1:F:198:GLU:CD	2.18	0.46
1:B:140:THR:HG1	1:B:198:GLU:CD	2.18	0.46
1:C:246:MET:HE1	1:C:251:ILE:CG1	2.42	0.46
3:L:19:DA:C2'	3:L:20:DC:H5''	2.46	0.46
1:F:136:GLN:HB3	1:F:139:LYS:HG3	1.97	0.46
2:I:6:DA:H2'	2:I:7:DA:C8	2.51	0.45
1:B:158:ARG:HG2	1:B:256:THR:OG1	2.16	0.45
1:D:117:GLY:O	1:D:118:THR:OG1	2.26	0.45
1:D:174:ARG:NH2	1:D:192:GLN:OE1	2.49	0.45
2:I:10:DT:C4	3:J:21:DA:N1	2.84	0.45
1:D:282:TRP:CE2	1:D:286:GLU:OE1	2.70	0.45
1:E:136:GLN:HB3	1:E:139:LYS:HG3	1.97	0.45
2:K:9:DA:C2	3:L:23:DG:C2	3.04	0.45
1:C:207:ASP:OD2	1:G:214:HIS:HE1	1.99	0.45
1:D:113:PHE:CD1	1:D:126:TYR:CE2	3.05	0.45
1:D:175:ARG:NH2	1:D:179:HIS:HB3	2.32	0.45
1:E:113:PHE:CD1	1:E:126:TYR:CE2	3.05	0.45
2:K:9:DA:N6	3:L:21:DA:N6	2.63	0.45
1:A:243:MET:HE2	1:C:179:HIS:CE1	2.52	0.45
1:B:175:ARG:HD3	1:B:191:PRO:O	2.17	0.44
3:J:20:DC:H1'	3:J:21:DA:H5''	1.99	0.44
1:E:282:TRP:CE2	1:E:286:GLU:OE1	2.71	0.44
1:C:174:ARG:NH2	1:C:192:GLN:OE1	2.50	0.44
1:A:282:TRP:CE2	1:A:286:GLU:OE1	2.70	0.44
1:C:209:ARG:N	1:G:174:ARG:HH22	2.15	0.44
1:A:113:PHE:CD1	1:A:126:TYR:CE2	3.06	0.44
1:G:113:PHE:CD1	1:G:126:TYR:CE2	3.06	0.44
1:B:113:PHE:CD1	1:B:126:TYR:CE2	3.06	0.44
1:C:209:ARG:CA	1:G:174:ARG:HH21	2.31	0.44
1:G:174:ARG:NH1	1:G:192:GLN:CG	2.79	0.44
1:C:175:ARG:HD3	1:C:191:PRO:O	2.18	0.44
1:C:209:ARG:CA	1:G:174:ARG:NH2	2.80	0.44
1:A:175:ARG:HD3	1:A:191:PRO:O	2.18	0.43
1:E:163:TYR:CZ	1:E:249:ARG:NH1	2.84	0.43
1:F:113:PHE:CD1	1:F:126:TYR:CE2	3.06	0.43
1:H:291:LYS:HG3	1:H:292:LYS:H	1.84	0.43
3:J:7:DC:H2'	3:J:8:DA:C8	2.53	0.43
1:C:113:PHE:CD1	1:C:126:TYR:CE2	3.07	0.43
1:G:291:LYS:HG3	1:G:292:LYS:N	2.34	0.43
2:I:21:DG:H1'	2:I:22:DT:H5'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLY:O	1:B:101:LYS:NZ	2.51	0.43
1:F:175:ARG:HD3	1:F:191:PRO:O	2.19	0.43
3:J:7:DC:C2'	3:J:8:DA:C8	3.02	0.42
1:G:174:ARG:HH12	1:G:192:GLN:CD	2.22	0.42
3:J:19:DA:C2'	3:J:20:DC:H5''	2.48	0.42
2:K:21:DG:H1'	2:K:22:DT:H5'	2.00	0.42
1:A:290:ARG:CG	1:A:291:LYS:N	2.82	0.42
1:C:135:CYS:O	1:C:274:VAL:HA	2.20	0.42
1:F:113:PHE:CD1	1:F:126:TYR:CD2	3.07	0.42
2:K:6:DA:H2'	2:K:7:DA:C8	2.54	0.42
1:E:175:ARG:HD3	1:E:191:PRO:O	2.20	0.42
1:E:184:ASP:HB2	6:E:303:PEG:O1	2.19	0.42
1:H:135:CYS:O	1:H:274:VAL:HA	2.20	0.42
1:E:290:ARG:CG	1:E:291:LYS:N	2.82	0.42
1:H:174:ARG:NH2	1:H:192:GLN:CB	2.81	0.42
1:H:174:ARG:HH22	1:H:192:GLN:CG	2.33	0.42
1:A:112:GLY:O	1:A:144:GLN:HG2	2.20	0.42
1:A:135:CYS:O	1:A:274:VAL:HA	2.19	0.42
1:A:171:GLU:OE1	1:A:249:ARG:NH2	2.47	0.42
1:C:291:LYS:HG3	1:C:292:LYS:N	2.34	0.42
1:D:135:CYS:O	1:D:274:VAL:HA	2.20	0.42
3:J:11:DA:C2'	3:J:12:DT:H5'	2.50	0.41
1:G:206:LEU:HG	1:G:207:ASP:N	2.35	0.41
1:H:289:LEU:HD12	1:H:292:LYS:HE2	2.02	0.41
1:C:246:MET:HE3	1:C:251:ILE:CG2	2.38	0.41
1:E:107:TYR:CE2	1:E:151:PRO:HA	2.56	0.41
1:D:175:ARG:HH21	1:D:179:HIS:HB3	1.85	0.41
1:F:140:THR:OG1	1:F:198:GLU:CD	2.59	0.41
3:L:7:DC:C2'	3:L:8:DA:C8	3.04	0.41
3:L:27:DC:H2'	3:L:28:DT:H72	2.03	0.41
1:F:287:GLU:O	1:F:290:ARG:HG3	2.21	0.41
1:B:135:CYS:O	1:B:274:VAL:HA	2.21	0.41
1:G:135:CYS:O	1:G:274:VAL:HA	2.21	0.41
2:K:7:DA:H2''	2:K:8:DC:H5'	2.03	0.41
1:A:113:PHE:CD1	1:A:126:TYR:CD2	3.09	0.41
1:C:209:ARG:N	1:G:174:ARG:NH2	2.69	0.41
1:E:112:GLY:O	1:E:144:GLN:HG2	2.21	0.41
3:J:20:DC:H2''	3:J:21:DA:H5'	2.03	0.41
1:F:112:GLY:O	1:F:144:GLN:HG2	2.21	0.40
1:C:166:SER:HB2	1:D:140:THR:HG21	2.03	0.40
1:D:171:GLU:OE1	1:D:249:ARG:NH2	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:THR:OG1	1:G:198:GLU:CD	2.59	0.40
1:F:135:CYS:O	1:F:274:VAL:HA	2.21	0.40
1:B:112:GLY:O	1:B:144:GLN:HG2	2.22	0.40
1:B:140:THR:OG1	1:B:198:GLU:CD	2.60	0.40
1:D:168:HIS:CE1	1:D:249:ARG:HD3	2.56	0.40
1:D:291:LYS:HG3	1:D:292:LYS:H	1.86	0.40
1:E:135:CYS:O	1:E:274:VAL:HA	2.21	0.40
1:H:174:ARG:NH2	1:H:192:GLN:CD	2.74	0.40
1:H:107:TYR:CE2	1:H:151:PRO:HA	2.57	0.40
2:K:24:DG:N2	3:L:8:DA:C2	2.90	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	196/200 (98%)	193 (98%)	3 (2%)	0	100	100
1	B	196/200 (98%)	191 (97%)	5 (3%)	0	100	100
1	C	196/200 (98%)	190 (97%)	6 (3%)	0	100	100
1	D	196/200 (98%)	190 (97%)	6 (3%)	0	100	100
1	E	196/200 (98%)	192 (98%)	4 (2%)	0	100	100
1	F	195/200 (98%)	191 (98%)	4 (2%)	0	100	100
1	G	196/200 (98%)	191 (97%)	5 (3%)	0	100	100
1	H	196/200 (98%)	191 (97%)	5 (3%)	0	100	100
All	All	1567/1600 (98%)	1529 (98%)	38 (2%)	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	178/179 (99%)	176 (99%)	2 (1%)	73	92
1	B	178/179 (99%)	176 (99%)	2 (1%)	73	92
1	C	178/179 (99%)	176 (99%)	2 (1%)	73	92
1	D	178/179 (99%)	176 (99%)	2 (1%)	73	92
1	E	178/179 (99%)	175 (98%)	3 (2%)	60	86
1	F	177/179 (99%)	175 (99%)	2 (1%)	73	92
1	G	178/179 (99%)	176 (99%)	2 (1%)	73	92
1	H	178/179 (99%)	176 (99%)	2 (1%)	73	92
All	All	1423/1432 (99%)	1406 (99%)	17 (1%)	71	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	155	THR
1	B	100	GLN
1	B	155	THR
1	C	100	GLN
1	C	248	ARG
1	D	100	GLN
1	D	155	THR
1	E	100	GLN
1	E	155	THR
1	E	174	ARG
1	F	155	THR
1	F	248	ARG
1	G	100	GLN
1	G	167	GLN
1	H	100	GLN
1	H	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	193	HIS
1	A	210	ASN
1	B	104	GLN
1	B	144	GLN
1	B	193	HIS
1	B	210	ASN
1	C	178	HIS
1	C	193	HIS
1	C	210	ASN
1	C	214	HIS
1	D	104	GLN
1	D	115	HIS
1	D	193	HIS
1	D	210	ASN
1	D	214	HIS
1	E	193	HIS
1	E	210	ASN
1	F	104	GLN
1	F	193	HIS
1	F	210	ASN
1	G	144	GLN
1	G	193	HIS
1	G	210	ASN
1	G	214	HIS
1	H	104	GLN
1	H	178	HIS
1	H	193	HIS
1	H	210	ASN
1	H	214	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 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	$\# Z > 2$
6	PEG	E	303	-	6,6,6	0.54	0	5,5,5	0.37	0
6	PEG	F	303	-	6,6,6	0.63	0	5,5,5	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	E	303	-	-	2/4/4/4	-
6	PEG	F	303	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	303	PEG	C4-C3-O2-C2
6	E	303	PEG	O1-C1-C2-O2
6	F	303	PEG	O1-C1-C2-O2
6	E	303	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	303	PEG	1	0

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, 95th 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 ²)	Q<0.9
1	A	198/200 (99%)	0.05	4 (2%) 65 63	51, 76, 117, 144	0
1	B	198/200 (99%)	0.07	3 (1%) 73 73	55, 78, 127, 160	0
1	C	198/200 (99%)	0.24	12 (6%) 21 17	41, 81, 135, 163	0
1	D	198/200 (99%)	0.15	11 (5%) 24 20	52, 80, 130, 190	0
1	E	198/200 (99%)	0.03	2 (1%) 82 82	51, 79, 120, 140	0
1	F	197/200 (98%)	0.09	5 (2%) 57 55	53, 82, 131, 164	0
1	G	198/200 (99%)	0.32	9 (4%) 33 29	49, 85, 134, 163	0
1	H	198/200 (99%)	0.29	12 (6%) 21 17	51, 84, 131, 171	0
2	I	30/30 (100%)	0.07	2 (6%) 17 13	33, 60, 118, 145	0
2	K	30/30 (100%)	0.14	3 (10%) 7 5	37, 72, 140, 164	0
3	J	30/30 (100%)	-0.06	4 (13%) 3 2	31, 73, 109, 141	0
3	L	30/30 (100%)	0.40	6 (20%) 1 0	41, 79, 163, 189	0
All	All	1703/1720 (99%)	0.15	73 (4%) 35 31	31, 80, 130, 190	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	117	GLY	8.3
1	H	118	THR	8.0
2	K	30	DG	7.4
1	D	119	ALA	6.7
2	K	29	DA	6.5
3	L	2	DT	6.0
2	I	29	DA	5.6
3	L	3	DC	5.5
1	C	120	LYS	5.1
1	C	225	VAL	4.6
1	G	120	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	121	SER	4.5
3	J	1	DC	4.4
1	G	121	SER	4.4
1	H	120	LYS	4.3
1	C	118	THR	4.0
1	D	121	SER	4.0
1	H	119	ALA	4.0
2	I	30	DG	3.8
1	D	118	THR	3.6
1	G	221	GLU	3.5
1	G	118	THR	3.4
1	C	119	ALA	3.4
1	E	95	SER	3.4
1	D	116	SER	3.2
1	D	120	LYS	3.2
1	E	236	TYR	3.2
3	J	2	DT	3.2
1	C	111	LEU	3.1
1	H	234	TYR	3.1
3	L	1	DC	3.1
1	F	262	GLY	3.1
1	G	201	LEU	3.0
3	L	4	DG	3.0
1	B	225	VAL	2.9
1	A	117	GLY	2.8
1	G	117	GLY	2.8
1	H	121	SER	2.8
1	D	157	VAL	2.8
1	H	268	ASN	2.7
1	C	188	LEU	2.7
1	D	95	SER	2.7
1	A	234	TYR	2.7
1	H	272	VAL	2.7
1	C	146	TRP	2.7
1	B	95	SER	2.6
3	J	30	DG	2.6
1	G	225	VAL	2.5
1	H	206	LEU	2.5
1	F	118	THR	2.5
1	D	134	PHE	2.4
1	C	187	GLY	2.4
3	J	3	DC	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	234	TYR	2.4
1	G	111	LEU	2.3
1	C	224	GLU	2.3
1	C	157	VAL	2.3
1	A	236	TYR	2.3
3	L	30	DG	2.3
1	A	95	SER	2.2
1	H	100	GLN	2.2
3	L	5	DA	2.2
1	G	119	ALA	2.2
1	D	111	LEU	2.1
1	H	255	ILE	2.1
1	D	207	ASP	2.1
1	F	243	MET	2.1
1	F	201	LEU	2.1
2	K	1	DC	2.0
1	C	291	LYS	2.0
1	F	107	TYR	2.0
1	D	115	HIS	2.0
1	H	115	HIS	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, 95th 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 ²)	Q<0.9
4	ARS	G	301	1/1	0.65	0.09	195,195,195,195	0
6	PEG	E	303	7/7	0.77	0.22	89,98,106,112	0
4	ARS	A	301	1/1	0.78	0.07	185,185,185,185	0

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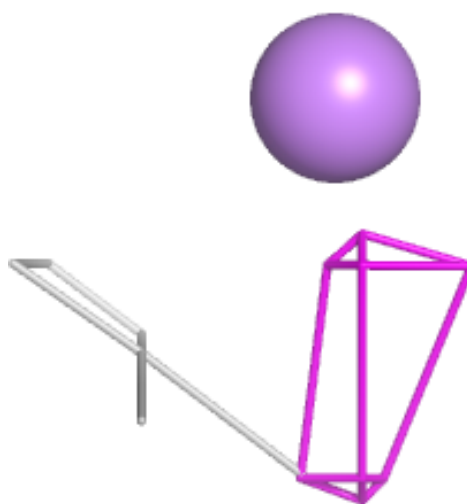
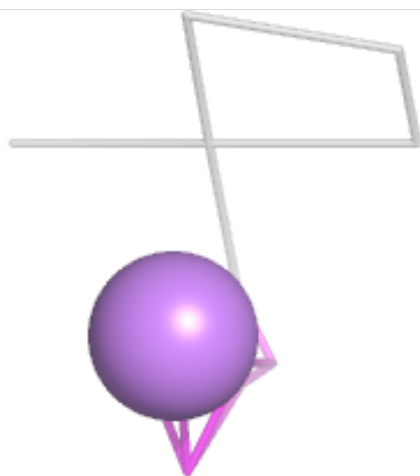
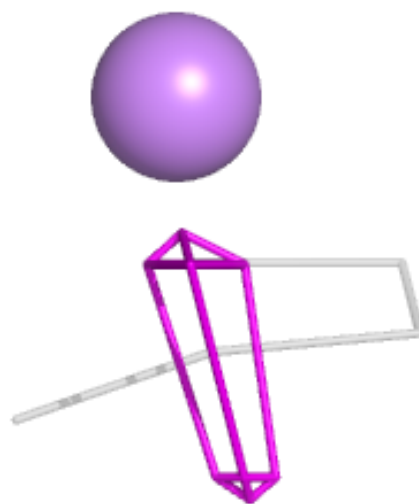
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ARS	F	301	1/1	0.78	0.08	191,191,191,191	0
4	ARS	E	301	1/1	0.84	0.10	188,188,188,188	0
6	PEG	F	303	7/7	0.86	0.20	74,84,101,101	0
4	ARS	C	301	1/1	0.87	0.05	178,178,178,178	0
4	ARS	B	301	1/1	0.88	0.07	161,161,161,161	0
4	ARS	D	301	1/1	0.89	0.10	176,176,176,176	0
4	ARS	H	301	1/1	0.90	0.08	172,172,172,172	0
5	ZN	D	302	1/1	0.95	0.17	65,65,65,65	0
5	ZN	E	302	1/1	0.96	0.21	70,70,70,70	0
5	ZN	B	302	1/1	0.97	0.18	69,69,69,69	0
5	ZN	H	302	1/1	0.99	0.20	68,68,68,68	0
5	ZN	A	302	1/1	0.99	0.22	71,71,71,71	0
5	ZN	G	302	1/1	0.99	0.21	64,64,64,64	0
5	ZN	C	302	1/1	1.00	0.19	60,60,60,60	0
5	ZN	F	302	1/1	1.00	0.15	66,66,66,66	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.

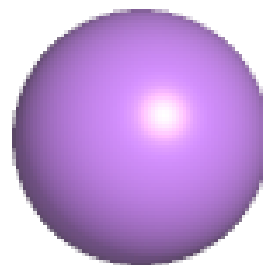
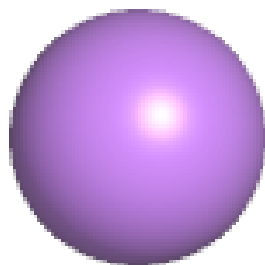
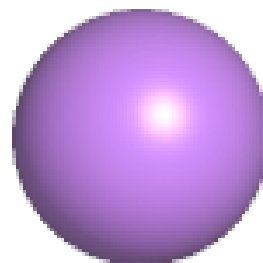
Electron density around ARS G 301:

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



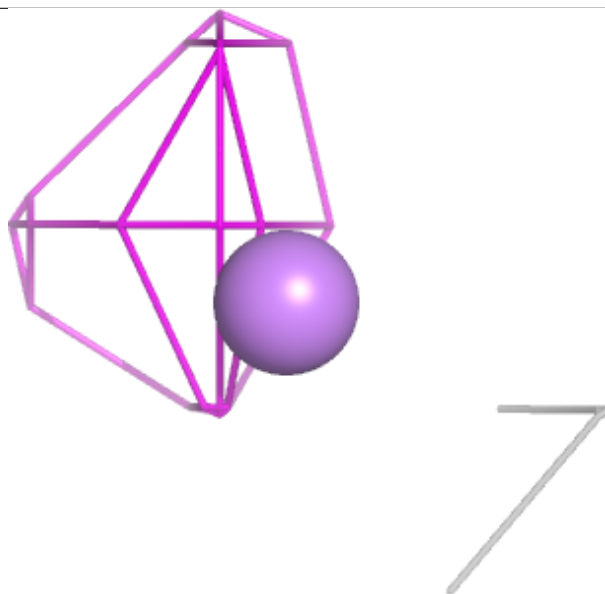
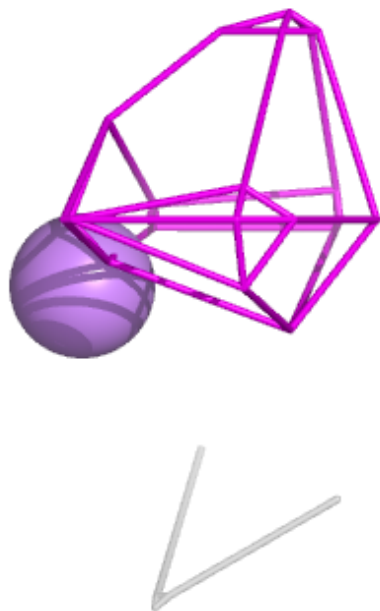
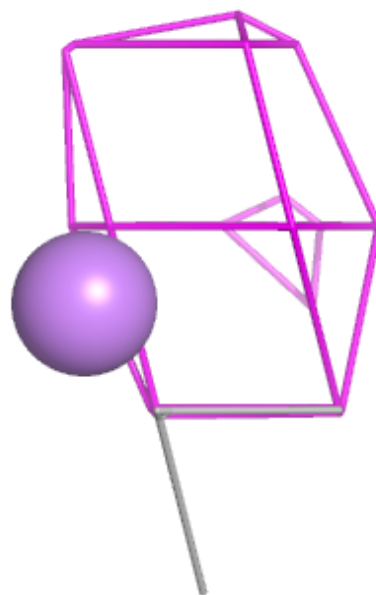
Electron density around ARS A 301:

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



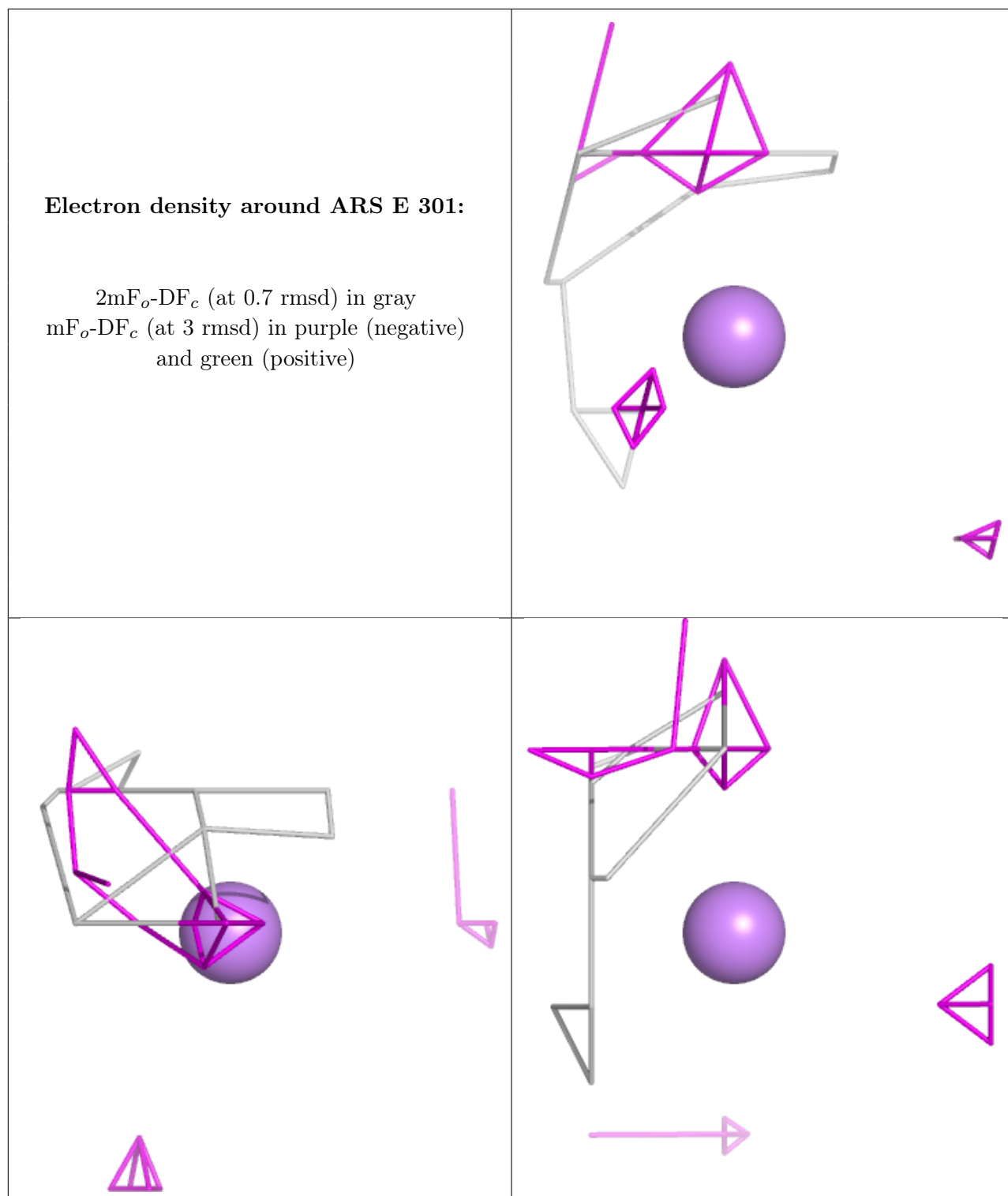
Electron density around ARS F 301:

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



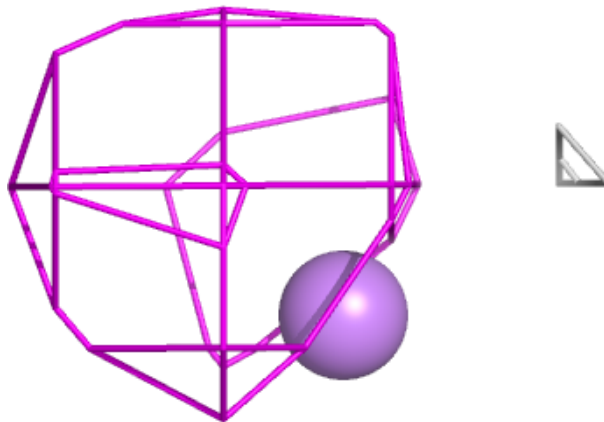
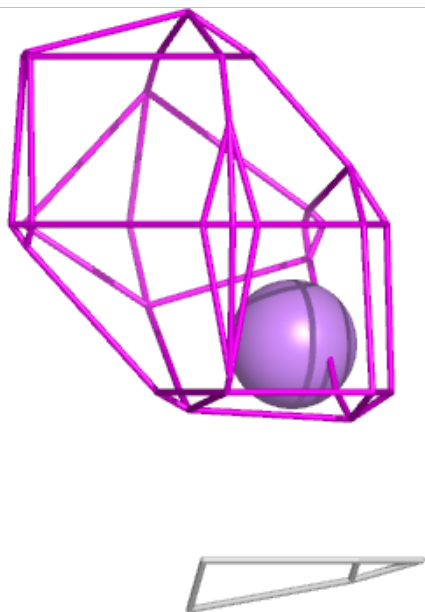
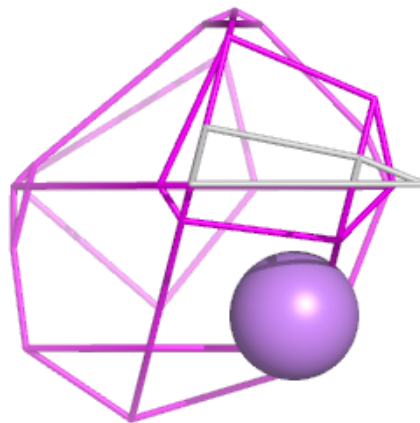
Electron density around ARS E 301:

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



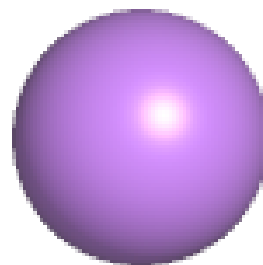
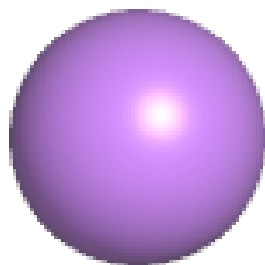
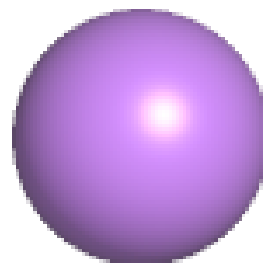
Electron density around ARS C 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



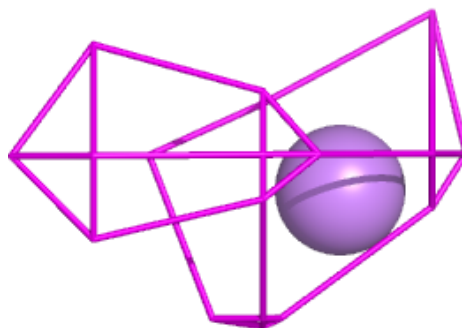
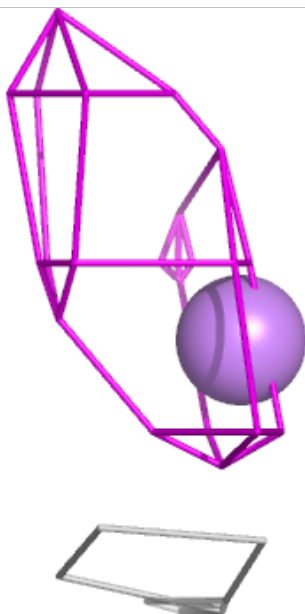
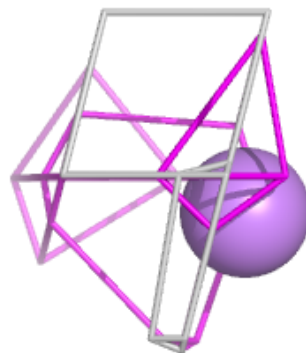
Electron density around ARS B 301:

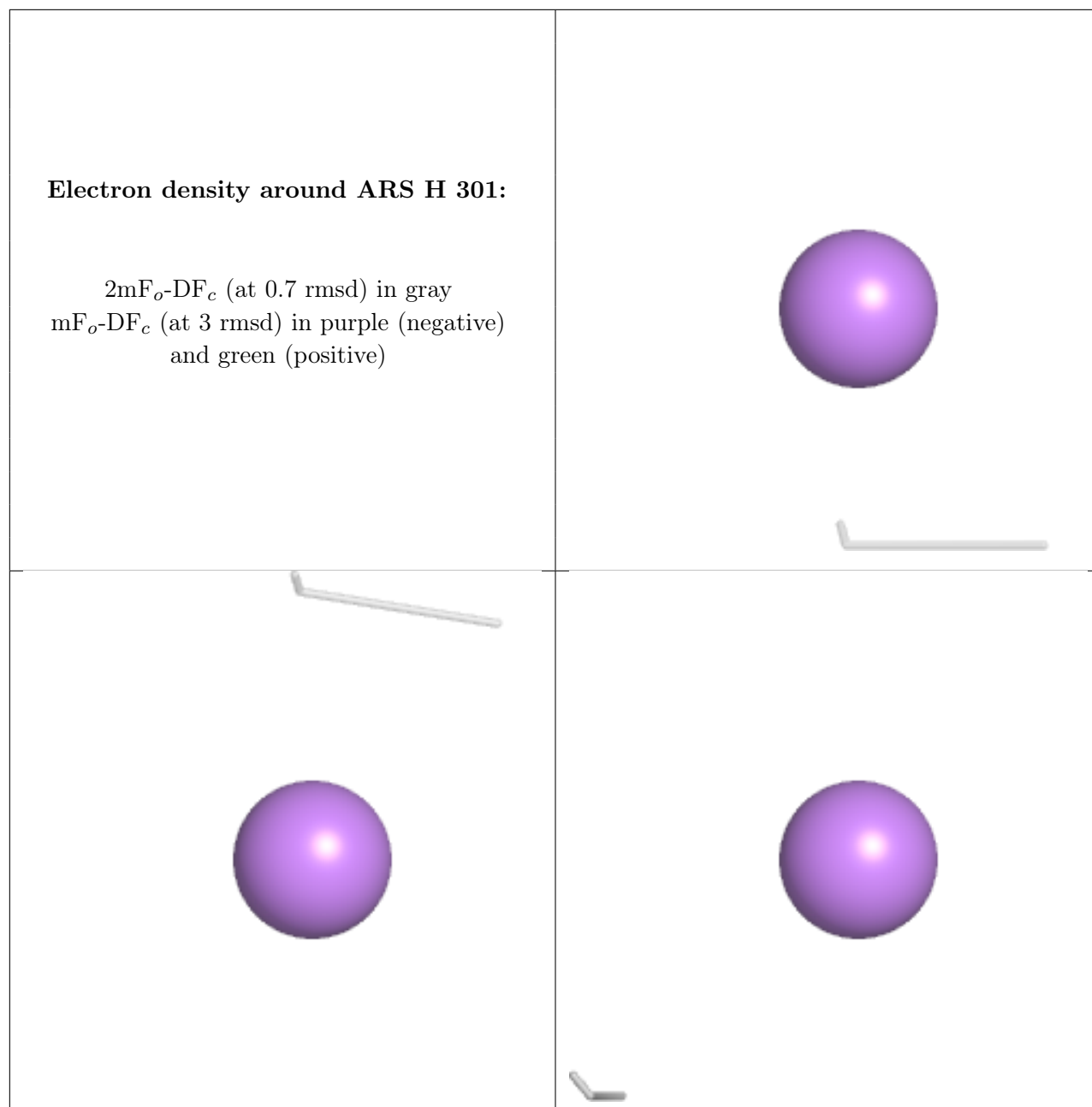
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ARS D 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 ⓘ

There are no such residues in this entry.