



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:26 PM UTC

PDB ID : 7EEU / pdb_00007eeu
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

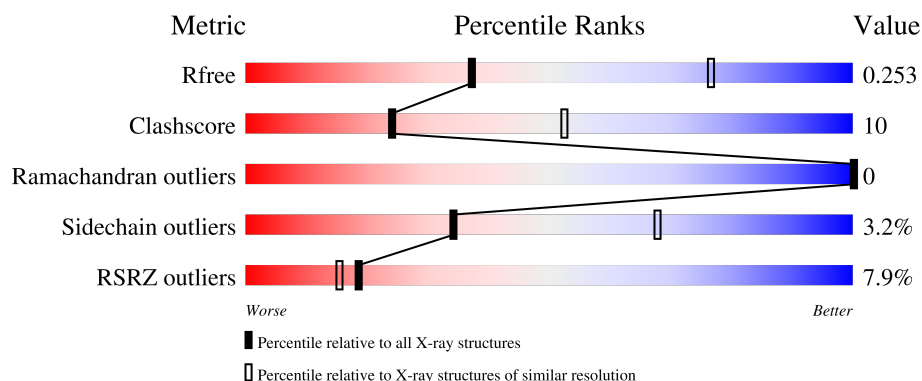
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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	8% 82% 16% .
1	B	200	8% 80% 18% .
1	C	200	8% 80% 19% .
1	D	200	9% 80% 17% ..
1	E	200	6% 78% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	200	4% 81% 16%
1	G	200	12% 80% 18%
1	H	200	12% 78% 21%
2	I	30	50% 40% 10%
2	K	30	3% 47% 50%
3	J	30	57% 37% 7%
3	L	30	3% 50% 47%

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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

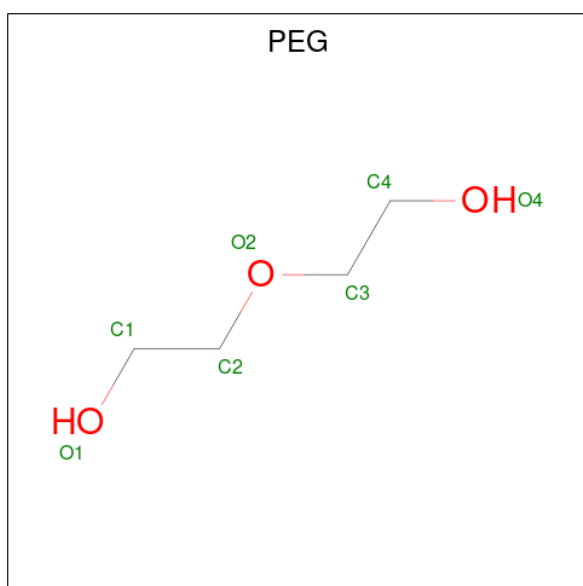
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

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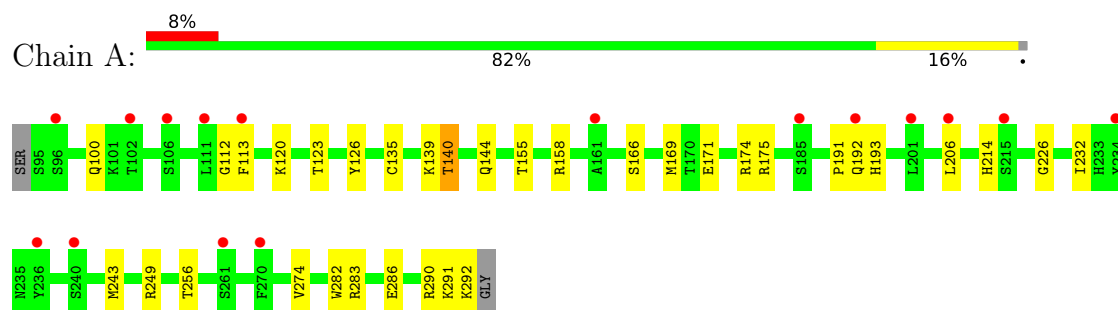
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total 2	O 2	0	0
7	D	2	Total 2	O 2	0	0
7	E	2	Total 2	O 2	0	0
7	F	1	Total 1	O 1	0	0
7	G	2	Total 2	O 2	0	0
7	H	1	Total 1	O 1	0	0
7	K	1	Total 1	O 1	0	0

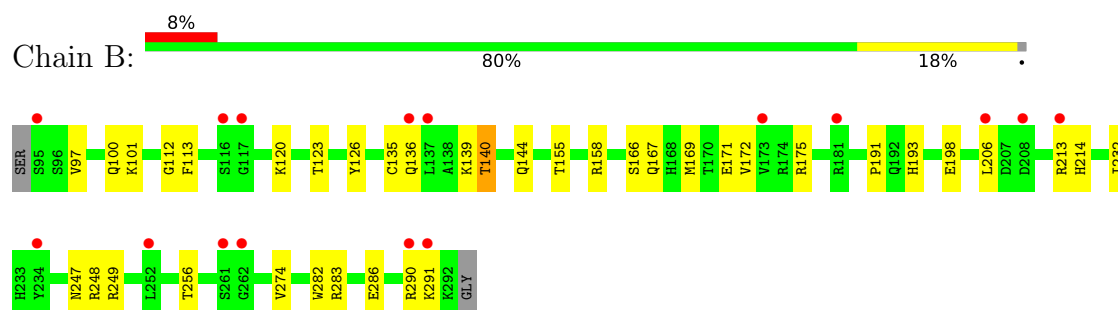
3 Residue-property plots

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.

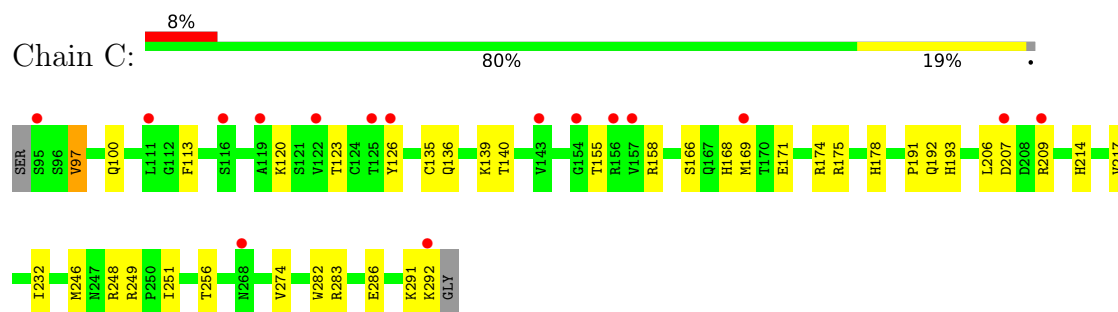
• Molecule 1: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53

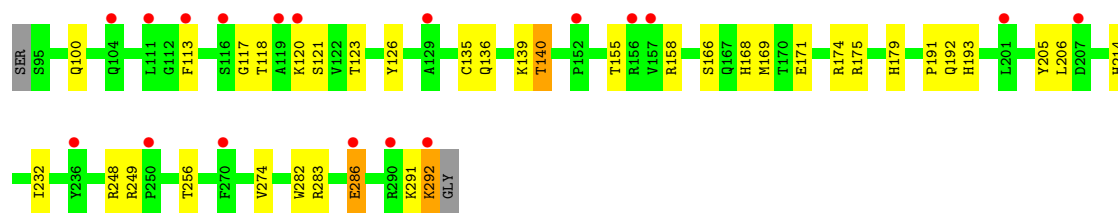


• Molecule 1: Cellular tumor antigen p53

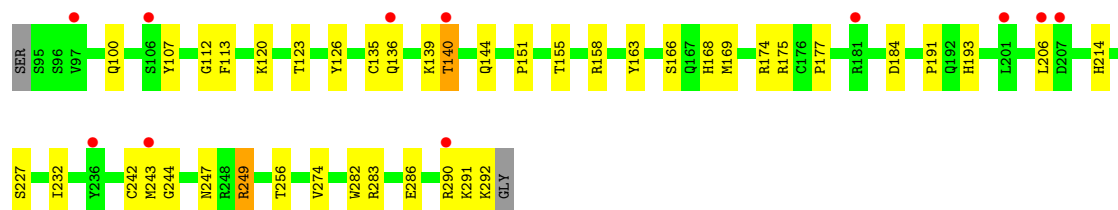
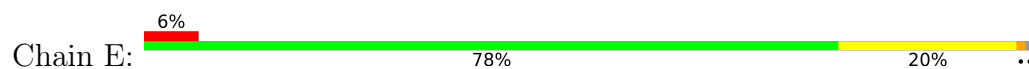


• Molecule 1: Cellular tumor antigen p53

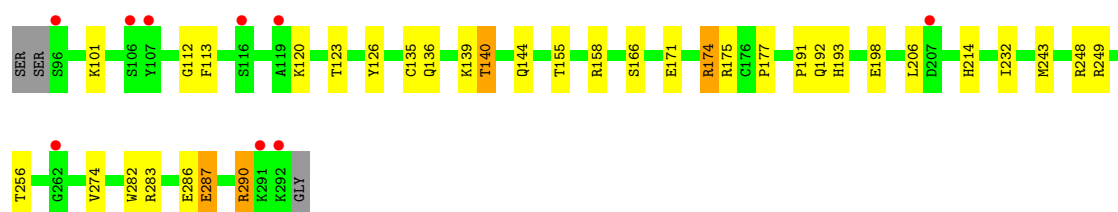
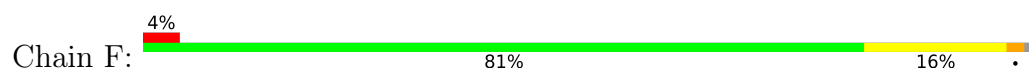




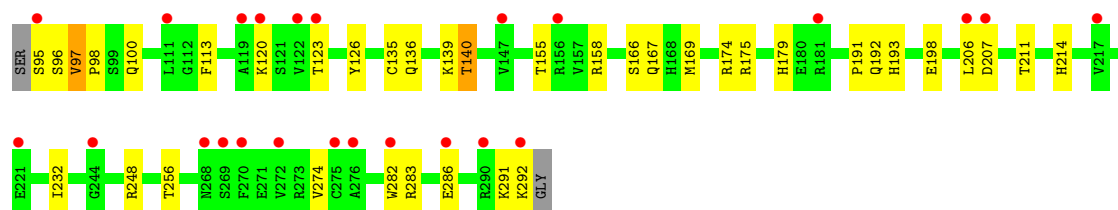
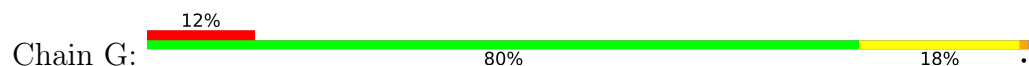
• Molecule 1: Cellular tumor antigen p53



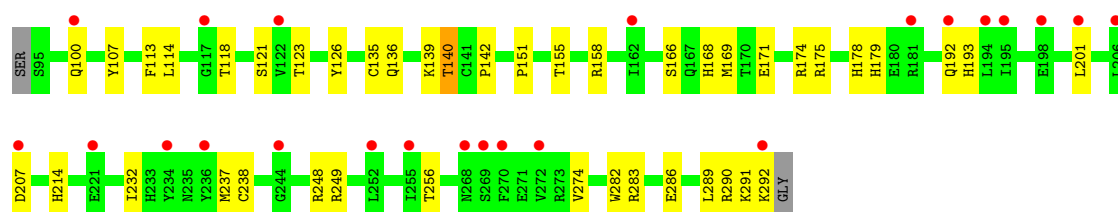
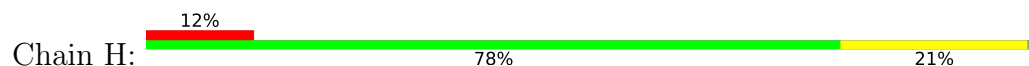
• Molecule 1: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53



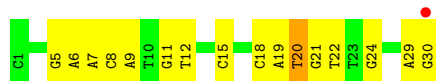
- Molecule 2: CDKN1A(p21) sense strand

Chain I:  50% 40% 10%



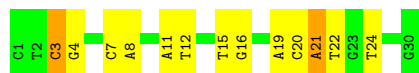
- Molecule 2: CDKN1A(p21) sense strand

Chain K:  3% 47% 50%



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

Chain J:  57% 37% 7%



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

Chain L:  3% 50% 47%



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 45.39 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.8 (45.39-2.90) 97.0 (45.39-2.90)	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 0.225 , 0.253	Depositor DCC
R_{free} test set	2948 reflections (4.94%)	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)	0.30 , 73.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PEG, ARS

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	0.85	0/1598	0.91	0/2166
1	B	0.81	0/1598	0.92	0/2166
1	C	0.82	1/1598 (0.1%)	0.90	0/2166
1	D	0.83	0/1598	0.90	0/2166
1	E	0.82	0/1598	0.92	1/2166 (0.0%)
1	F	0.82	0/1592	0.92	2/2158 (0.1%)
1	G	0.78	0/1598	0.90	1/2166 (0.0%)
1	H	0.78	0/1598	0.94	2/2166 (0.1%)
2	I	0.53	0/691	1.00	4/1064 (0.4%)
2	K	0.46	0/691	0.96	4/1064 (0.4%)
3	J	0.54	0/687	1.06	4/1058 (0.4%)
3	L	0.46	0/687	1.01	3/1058 (0.3%)
All	All	0.77	1/15534 (0.0%)	0.93	21/21564 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	VAL	CA-CB	-5.07	1.50	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	19	DA	C4'-C3'-O3'	-7.60	98.61	110.00
2	K	18	DC	C4'-C3'-O3'	-7.24	99.14	110.00
2	I	18	DC	C4'-C3'-O3'	-6.89	99.67	110.00
2	K	19	DA	C4'-C3'-O3'	-6.88	99.69	110.00
2	I	20	DT	C4'-C3'-O3'	-6.59	100.11	110.00
1	F	174	ARG	N-CA-CB	-6.16	101.64	111.43
2	K	20	DT	C4'-C3'-O3'	-6.08	100.88	110.00
2	I	9	DA	C4'-C3'-O3'	-5.75	101.38	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	24	DT	C4'-C3'-O3'	-5.69	101.46	110.00
3	J	21	DA	C2'-C3'-O3'	-5.47	103.29	111.50
1	E	249	ARG	CG-CD-NE	5.44	123.97	112.00
1	F	287	GLU	CB-CG-CD	5.42	121.82	112.60
3	L	3	DC	C2'-C3'-O3'	-5.38	103.43	111.50
3	J	24	DT	C4'-C3'-O3'	-5.36	101.96	110.00
3	J	24	DT	C2'-C3'-O3'	5.25	119.38	111.50
1	H	290	ARG	CB-CG-CD	5.20	123.25	111.30
1	H	118	THR	N-CA-C	5.19	117.01	111.36
1	G	97	VAL	N-CA-C	5.14	119.99	108.88
2	K	18	DC	C2'-C3'-O3'	5.14	119.21	111.50
3	J	3	DC	C2'-C3'-O3'	-5.10	103.85	111.50
3	L	24	DT	C2'-C3'-O3'	5.08	119.12	111.50

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	36	0
1	D	1561	0	1518	25	0
1	E	1561	0	1518	27	0
1	F	1555	0	1513	28	0
1	G	1561	0	1518	43	0
1	H	1561	0	1518	35	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
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	264	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 (264) 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:C:246:MET:HE3	1:C:251:ILE:HG23	1.31	1.08
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
1:C:246:MET:HE3	1:C:251:ILE:CG2	1.94	0.97
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
2:I:20:DT:N3	3:J:11:DA:N1	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:243:MET:HE2	1:C:178:HIS:HD2	1.45	0.79
1:H:175:ARG:HE	1:H:179:HIS:HB3	1.46	0.79
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:G:174:ARG:NH1	1:G:192:GLN:CD	2.48	0.72
1:A:243:MET:HE2	1:C:178:HIS:CD2	2.24	0.72
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:B:120:LYS:HD2	3:J:7:DC:C5'	2.22	0.69
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:E:243:MET:O	1:E:243:MET:HG2	1.96	0.64
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:D:205:TYR:C	1:D:206:LEU:HD22	2.24	0.63
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
1:C:192:GLN:NE2	1:G:206:LEU:HD11	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:291:LYS:O	1:H:292:LYS:C	2.50	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:H:174:ARG:HH22	1:H:192:GLN:CD	2.16	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
1:F:136:GLN:HB3	1:F:139:LYS:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:117:GLY:O	1:D:118:THR:OG1	2.26	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:G:140:THR:HG1	1:G:198:GLU:CD	2.20	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:C:246:MET:HE3	1:C:251:ILE:HG21	1.89	0.49
1:D:192:GLN:OE1	1:H:207:ASP:O	2.30	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: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:B:140:THR:HG1	1:B:198:GLU:CD	2.21	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:F:140:THR:HG1	1:F:198:GLU:CD	2.22	0.47
1:G:174:ARG:HH12	1:G:192:GLN:CD	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:SER:O	1:G:98:PRO:HD3	2.16	0.46
1:B:136:GLN:HB3	1:B:139:LYS:HG3	1.96	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:F:140:THR:OG1	1:F:198:GLU:CD	2.59	0.45
1:B:158:ARG:HG2	1:B:256:THR:OG1	2.16	0.45
1:D:174:ARG:NH2	1:D:192:GLN:OE1	2.49	0.45
1:G:140:THR:OG1	1:G:198:GLU:CD	2.59	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:B:140:THR:OG1	1:B:198:GLU:CD	2.60	0.45
1:C:207:ASP:OD2	1:G:214:HIS:HE1	1.99	0.45
1:H:174:ARG:NH2	1:H:192:GLN:CD	2.74	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: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
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:H:168:HIS:O	1:H:169:MET:C	2.63	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
1:E:168:HIS:O	1:E:169:MET:C	2.63	0.41
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: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
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:C:168:HIS:O	1:C:169:MET:C	2.64	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:C:246:MET:HE1	1:C:251:ILE:HG12	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLU:OE1	1:D:249:ARG:NH2	2.43	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: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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	173 (97%)	5 (3%)	38	72
1	B	178/179 (99%)	173 (97%)	5 (3%)	38	72
1	C	178/179 (99%)	173 (97%)	5 (3%)	38	72
1	D	178/179 (99%)	171 (96%)	7 (4%)	28	63
1	E	178/179 (99%)	172 (97%)	6 (3%)	32	66
1	F	177/179 (99%)	171 (97%)	6 (3%)	32	66
1	G	178/179 (99%)	172 (97%)	6 (3%)	32	66
1	H	178/179 (99%)	172 (97%)	6 (3%)	32	66
All	All	1423/1432 (99%)	1377 (97%)	46 (3%)	34	68

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	140	THR
1	A	155	THR
1	A	232	ILE
1	A	292	LYS
1	B	100	GLN
1	B	140	THR
1	B	155	THR
1	B	232	ILE
1	B	248	ARG
1	C	100	GLN
1	C	140	THR
1	C	155	THR
1	C	232	ILE
1	C	248	ARG
1	D	100	GLN
1	D	140	THR
1	D	155	THR
1	D	232	ILE

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Mol	Chain	Res	Type
1	D	248	ARG
1	D	286	GLU
1	D	292	LYS
1	E	100	GLN
1	E	140	THR
1	E	155	THR
1	E	174	ARG
1	E	232	ILE
1	E	292	LYS
1	F	140	THR
1	F	155	THR
1	F	177	PRO
1	F	232	ILE
1	F	248	ARG
1	F	290	ARG
1	G	100	GLN
1	G	140	THR
1	G	155	THR
1	G	167	GLN
1	G	232	ILE
1	G	248	ARG
1	H	100	GLN
1	H	140	THR
1	H	155	THR
1	H	232	ILE
1	H	248	ARG
1	H	286	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	210	ASN
1	A	239	ASN
1	A	247	ASN
1	B	104	GLN
1	B	144	GLN
1	B	210	ASN
1	B	239	ASN
1	C	144	GLN
1	C	178	HIS
1	C	192	GLN

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Mol	Chain	Res	Type
1	C	210	ASN
1	C	214	HIS
1	C	239	ASN
1	D	104	GLN
1	D	115	HIS
1	D	178	HIS
1	D	210	ASN
1	D	214	HIS
1	D	239	ASN
1	D	247	ASN
1	E	144	GLN
1	E	210	ASN
1	E	239	ASN
1	F	104	GLN
1	F	210	ASN
1	F	239	ASN
1	G	144	GLN
1	G	210	ASN
1	G	214	HIS
1	G	239	ASN
1	H	104	GLN
1	H	178	HIS
1	H	210	ASN
1	H	214	HIS
1	H	239	ASN
1	H	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.55	0	5,5,5	0.37	0
6	PEG	F	303	-	6,6,6	0.64	0	5,5,5	0.73	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%)	0.85	16 (8%) 18 15	51, 76, 117, 144	0
1	B	198/200 (99%)	0.74	16 (8%) 18 15	55, 78, 127, 160	0
1	C	198/200 (99%)	0.71	16 (8%) 18 15	41, 81, 135, 163	0
1	D	198/200 (99%)	0.67	18 (9%) 15 12	52, 80, 130, 190	0
1	E	198/200 (99%)	0.78	11 (5%) 30 23	51, 79, 120, 140	0
1	F	197/200 (98%)	0.75	9 (4%) 37 29	53, 82, 131, 164	0
1	G	198/200 (99%)	0.84	24 (12%) 8 7	49, 85, 134, 163	0
1	H	198/200 (99%)	0.97	23 (11%) 9 8	51, 84, 131, 171	0
2	I	30/30 (100%)	0.07	0 100 100	33, 60, 118, 145	0
2	K	30/30 (100%)	0.42	1 (3%) 49 40	37, 72, 140, 164	0
3	J	30/30 (100%)	0.15	0 100 100	31, 73, 109, 141	0
3	L	30/30 (100%)	0.33	1 (3%) 49 40	41, 79, 163, 189	0
All	All	1703/1720 (99%)	0.75	135 (7%) 18 15	31, 80, 130, 190	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	SER	5.5
1	C	111	LEU	4.9
1	H	234	TYR	4.7
1	H	270	PHE	4.6
1	F	106	SER	4.1
1	H	268	ASN	4.0
1	G	268	ASN	4.0
1	H	272	VAL	3.9
1	G	206	LEU	3.7
1	B	234	TYR	3.6
1	D	270	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	255	ILE	3.5
1	B	95	SER	3.5
1	C	292	LYS	3.3
1	B	262	GLY	3.3
1	H	181	ARG	3.3
1	A	234	TYR	3.2
1	E	236	TYR	3.2
1	B	206	LEU	3.2
1	D	157	VAL	3.2
1	G	111	LEU	3.1
1	H	269	SER	3.1
1	G	292	LYS	3.1
1	H	195	ILE	3.1
1	A	185	SER	3.1
1	C	157	VAL	3.1
1	D	207	ASP	3.1
1	B	261	SER	3.0
1	G	269	SER	3.0
1	F	262	GLY	2.9
1	G	221	GLU	2.9
1	D	292	LYS	2.9
1	F	207	ASP	2.9
1	G	156	ARG	2.9
1	G	123	THR	2.9
1	E	136	GLN	2.8
1	H	194	LEU	2.8
1	A	206	LEU	2.8
1	F	291	LYS	2.8
1	B	208	ASP	2.7
1	E	207	ASP	2.7
1	G	95	SER	2.7
1	G	286	GLU	2.7
1	G	119	ALA	2.7
1	E	97	VAL	2.7
1	C	156	ARG	2.7
1	G	276	ALA	2.7
1	D	111	LEU	2.6
1	E	201	LEU	2.6
1	E	206	LEU	2.6
1	A	161	ALA	2.6
1	H	236	TYR	2.6
1	A	201	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	207	ASP	2.6
1	E	106	SER	2.6
1	D	250	PRO	2.6
1	F	107	TYR	2.6
1	G	272	VAL	2.6
1	A	192	GLN	2.6
1	D	236	TYR	2.5
1	B	291	LYS	2.5
1	E	140	THR	2.5
1	H	192	GLN	2.5
1	F	292	LYS	2.5
1	G	122	VAL	2.5
1	H	207	ASP	2.5
1	F	116	SER	2.5
1	A	96	SER	2.4
1	C	122	VAL	2.4
1	B	181	ARG	2.4
1	G	270	PHE	2.4
1	H	198	GLU	2.4
1	G	217	VAL	2.4
1	G	244	GLY	2.4
1	H	117	GLY	2.4
1	C	95	SER	2.4
3	L	3	DC	2.4
1	C	143	VAL	2.4
1	C	209	ARG	2.4
1	D	286	GLU	2.4
1	A	240	SER	2.4
1	A	236	TYR	2.4
1	D	120	LYS	2.3
1	H	162	ILE	2.3
1	C	268	ASN	2.3
1	H	252	LEU	2.3
1	B	117	GLY	2.3
1	D	113	PHE	2.3
1	B	116	SER	2.3
1	G	120	LYS	2.3
1	B	290	ARG	2.3
1	C	126	TYR	2.3
1	D	119	ALA	2.3
1	D	152	PRO	2.3
1	C	119	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	2.2
1	B	252	LEU	2.2
1	A	113	PHE	2.2
1	G	207	ASP	2.2
1	G	282	TRP	2.2
1	H	122	VAL	2.2
1	F	119	ALA	2.2
1	H	292	LYS	2.2
1	A	106	SER	2.2
1	D	201	LEU	2.2
1	B	213	ARG	2.1
1	D	156	ARG	2.1
1	H	100	GLN	2.1
1	C	116	SER	2.1
1	G	290	ARG	2.1
1	E	243	MET	2.1
1	C	125	THR	2.1
1	C	154	GLY	2.1
1	H	201	LEU	2.1
1	D	129	ALA	2.1
1	G	181	ARG	2.1
1	A	215	SER	2.1
1	F	96	SER	2.1
1	C	169	MET	2.1
1	G	147	VAL	2.1
1	B	137	LEU	2.1
1	H	206	LEU	2.1
1	H	244	GLY	2.1
1	B	136	GLN	2.1
1	B	173	VAL	2.1
1	E	290	ARG	2.1
1	H	221	GLU	2.1
1	D	104	GLN	2.0
1	A	102	THR	2.0
2	K	30	DG	2.0
1	D	116	SER	2.0
1	G	275	CYS	2.0
1	D	290	ARG	2.0
1	E	181	ARG	2.0
1	A	270	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

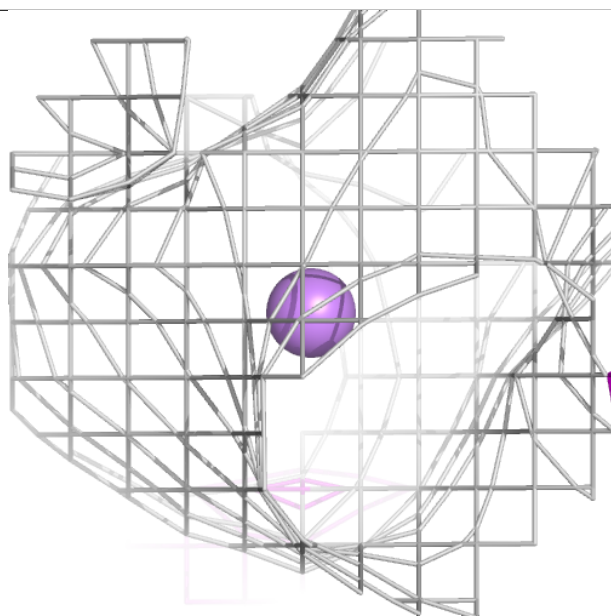
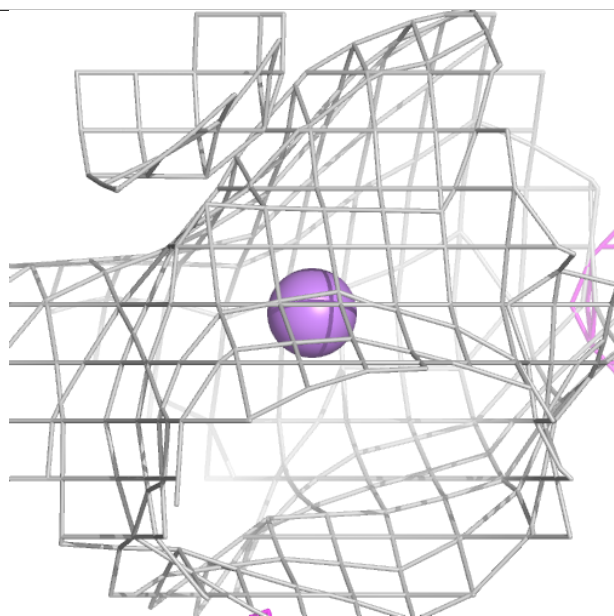
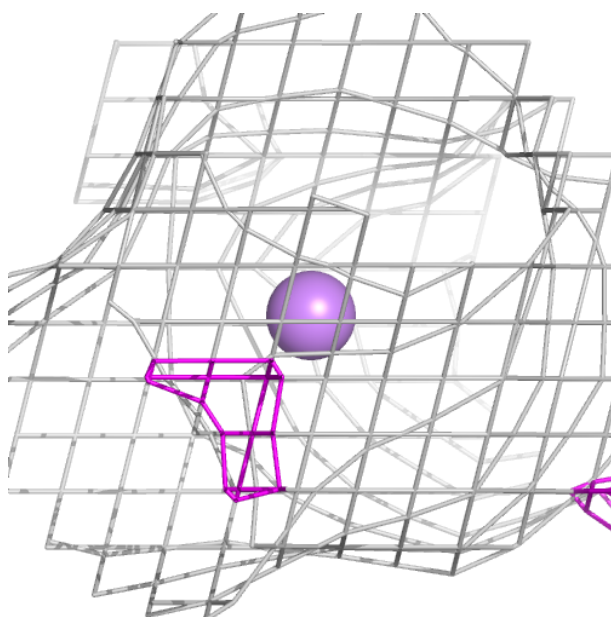
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	E	303	7/7	0.77	0.12	89,98,106,112	0
6	PEG	F	303	7/7	0.83	0.17	74,84,101,101	0
4	ARS	E	301	1/1	0.90	0.16	188,188,188,188	0
4	ARS	F	301	1/1	0.91	0.10	191,191,191,191	0
4	ARS	A	301	1/1	0.92	0.08	185,185,185,185	0
4	ARS	G	301	1/1	0.93	0.08	195,195,195,195	0
4	ARS	C	301	1/1	0.94	0.09	178,178,178,178	0
4	ARS	H	301	1/1	0.94	0.07	172,172,172,172	0
4	ARS	B	301	1/1	0.95	0.06	161,161,161,161	0
4	ARS	D	301	1/1	0.95	0.12	176,176,176,176	0
5	ZN	D	302	1/1	0.99	0.04	65,65,65,65	0
5	ZN	E	302	1/1	0.99	0.07	70,70,70,70	0
5	ZN	G	302	1/1	0.99	0.08	64,64,64,64	0
5	ZN	H	302	1/1	0.99	0.07	68,68,68,68	0
5	ZN	A	302	1/1	0.99	0.09	71,71,71,71	0
5	ZN	B	302	1/1	0.99	0.05	69,69,69,69	0
5	ZN	C	302	1/1	1.00	0.06	60,60,60,60	0
5	ZN	F	302	1/1	1.00	0.04	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.

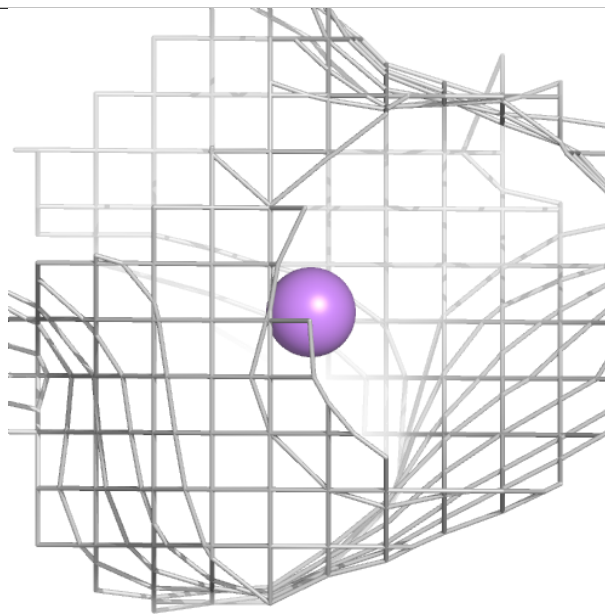
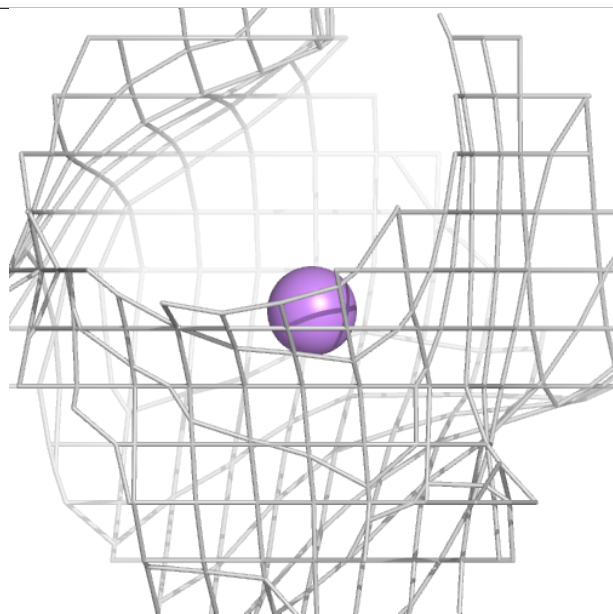
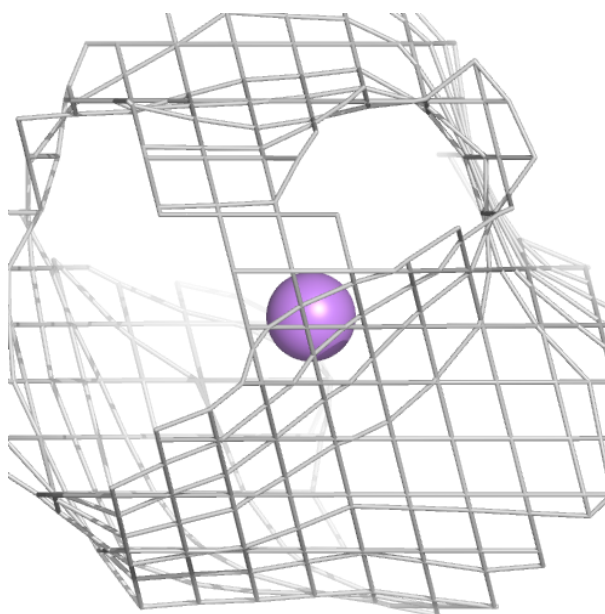
Electron density around ARS E 301:

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



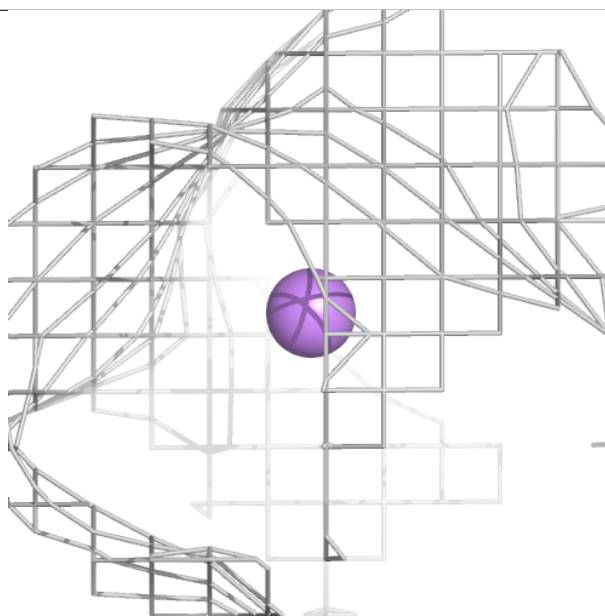
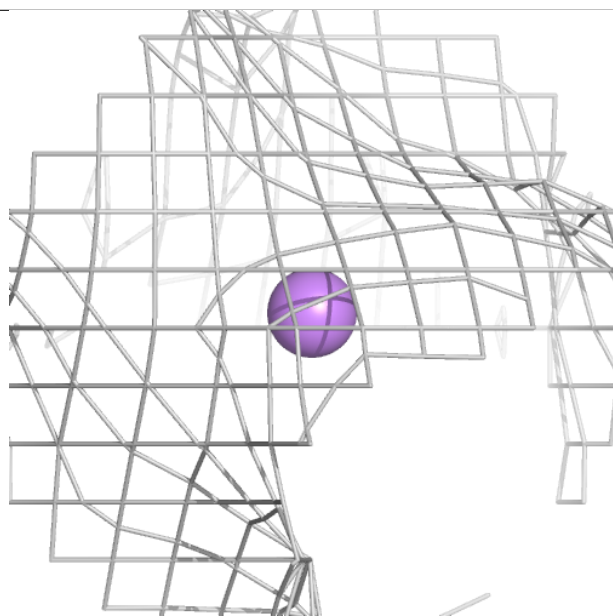
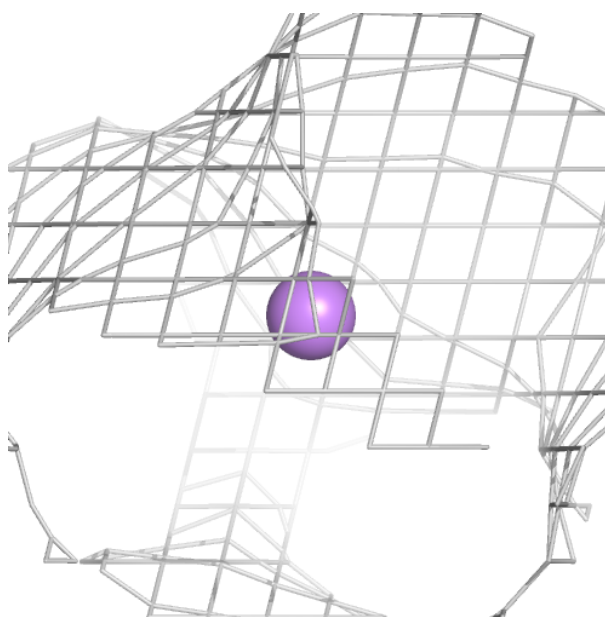
Electron density around ARS F 301:

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



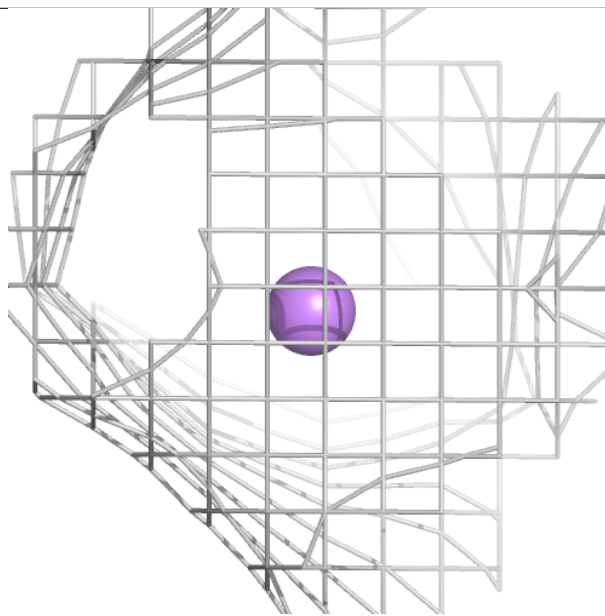
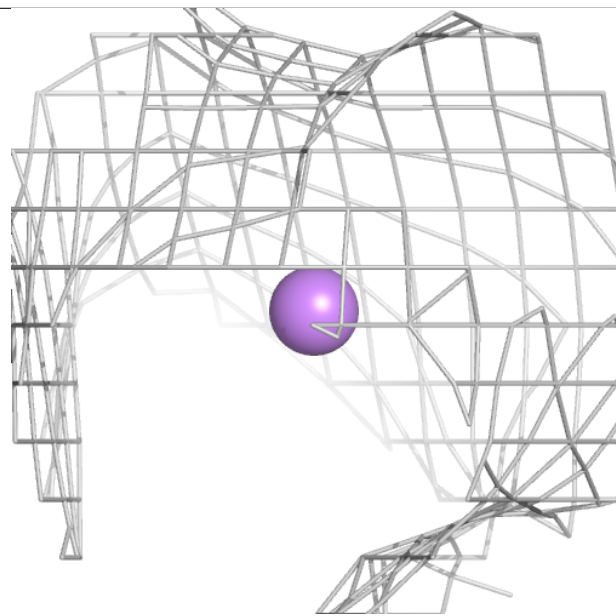
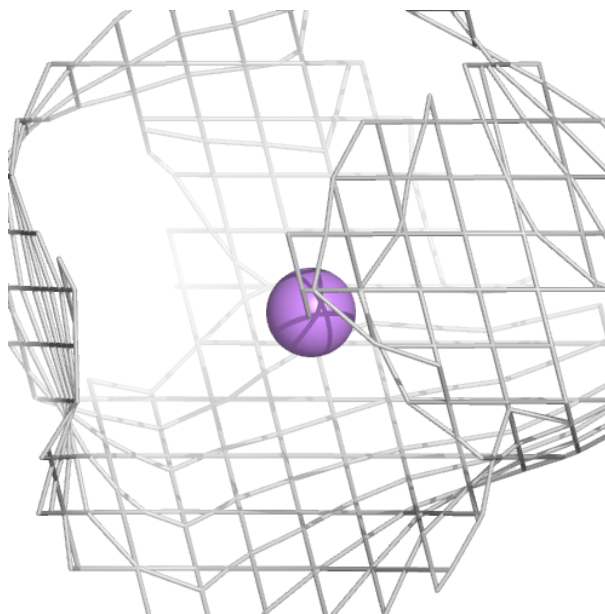
Electron density around ARS A 301:

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and green (positive)



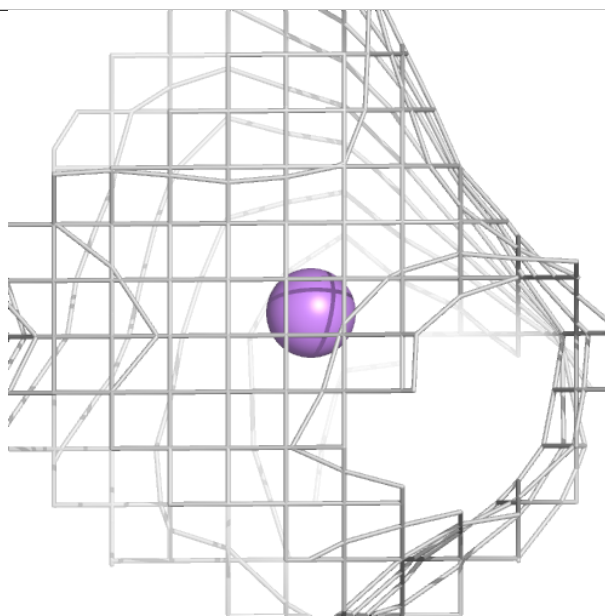
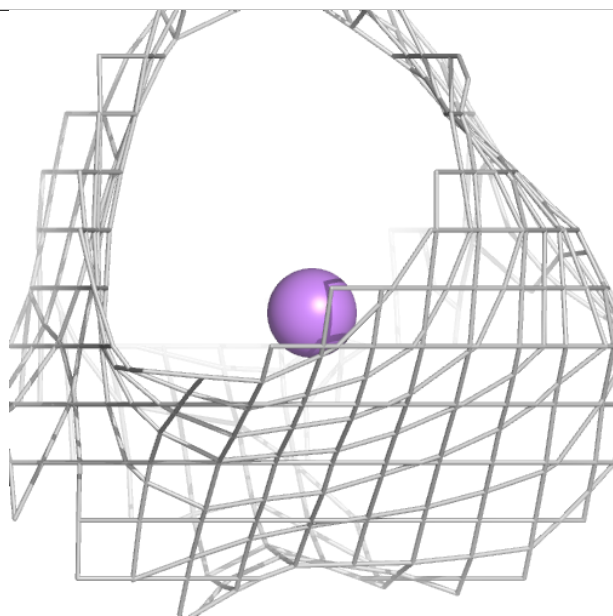
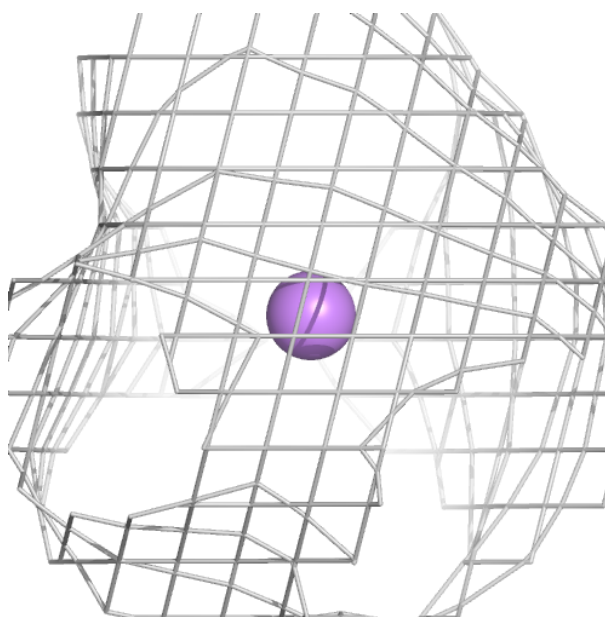
Electron density around ARS G 301:

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



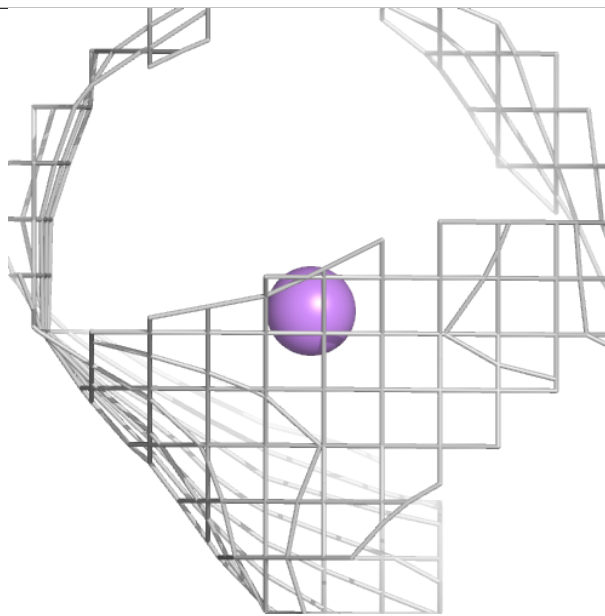
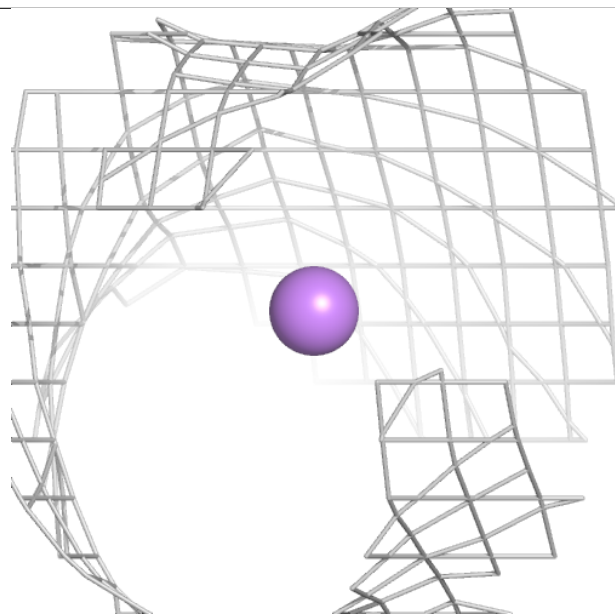
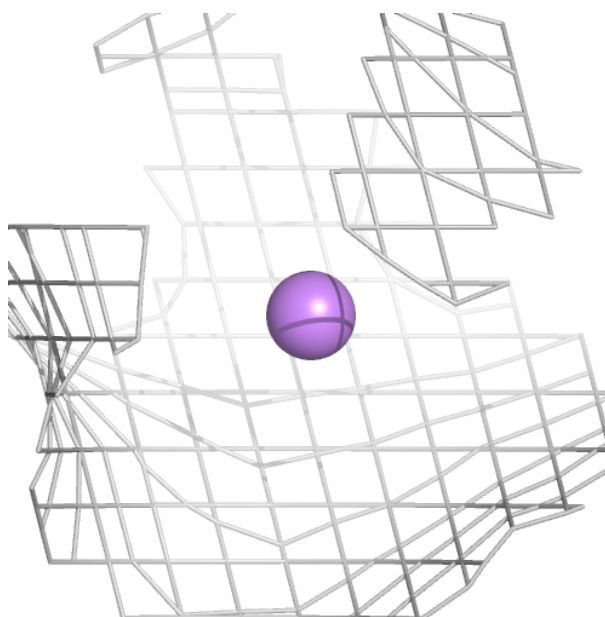
Electron density around ARS C 301:

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



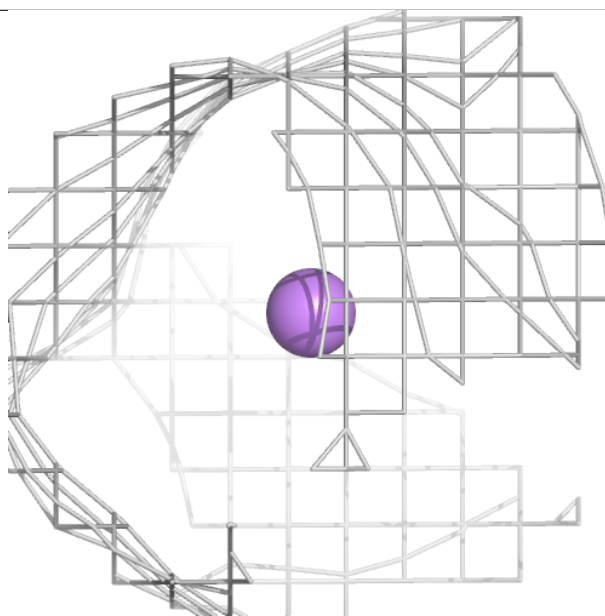
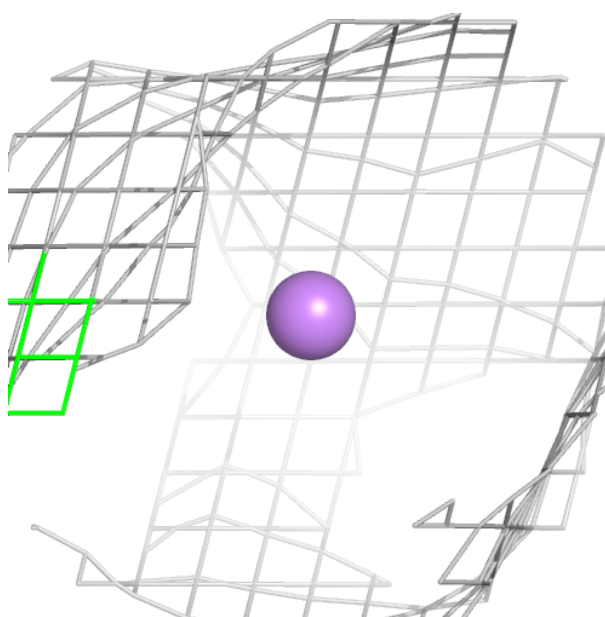
Electron density around ARS H 301:

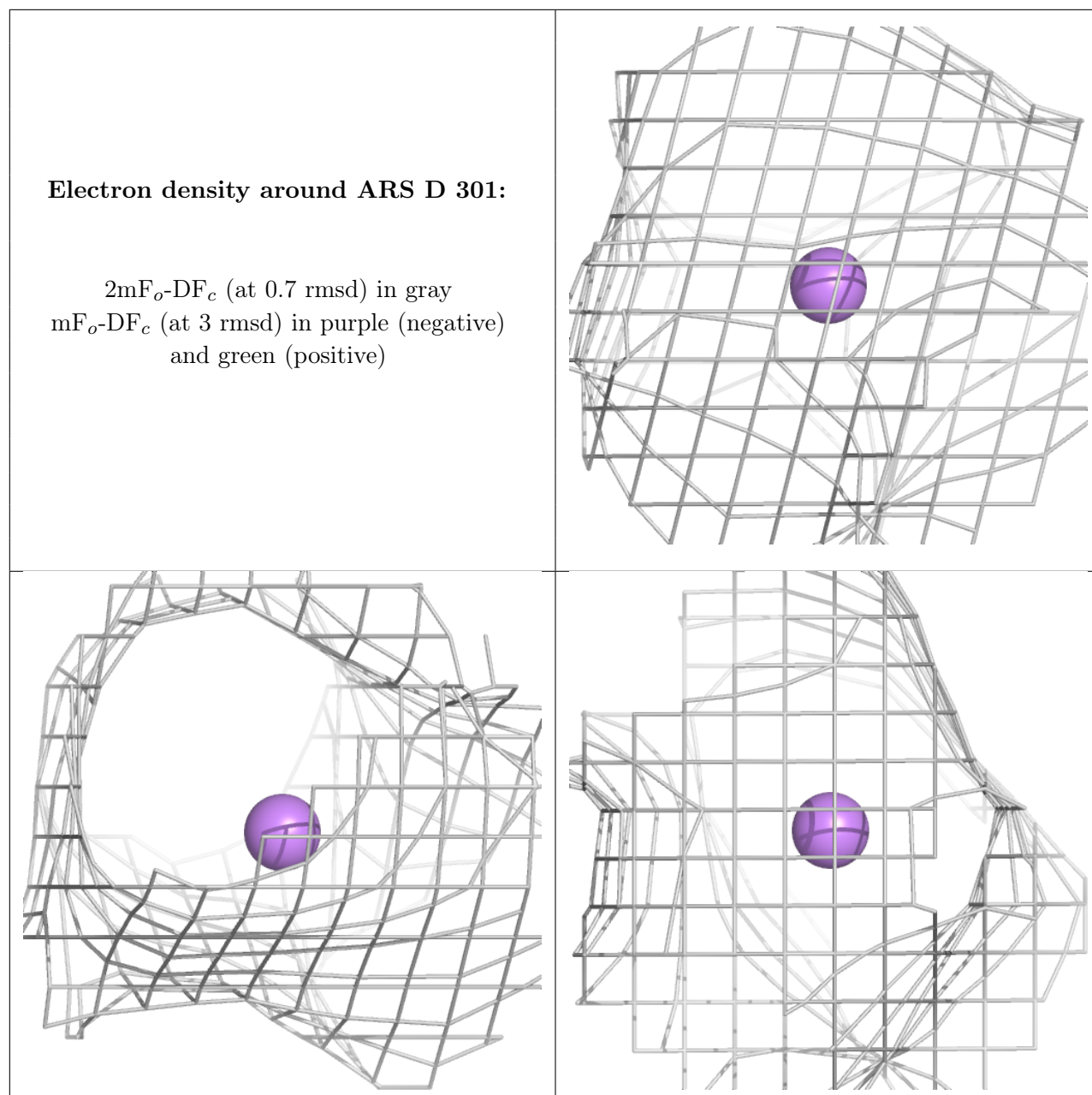
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ARS 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.