Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2024 – 12:34 pm GMT

PDB ID	:	8Q3X
Title	:	Structure of Nucleosome Core with a Bound Metallopeptide Conjugate (Kaposi Sarcoma Associated Herpesvirus LANA Peptide-Au[I] Compound)
Authors	:	De Falco, L.; Batchelor, L.K.; Dyson, P.J.; Davey, C.A.
Deposited on	:	2023-08-04
Resolution	:	2.30 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:

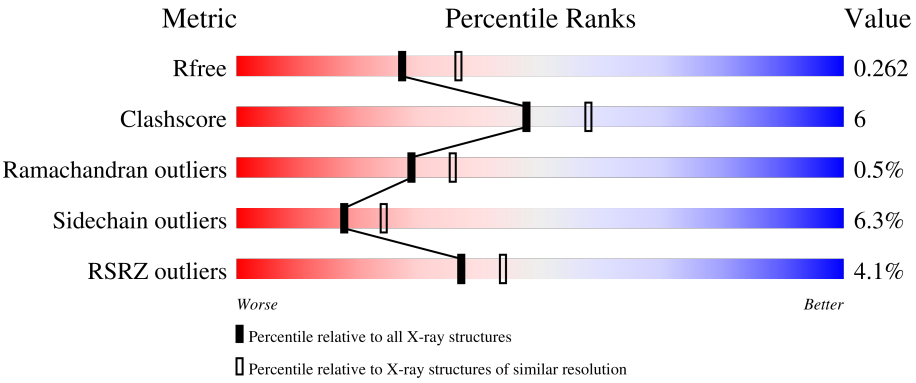
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	AAA	98	3% 89% 11%
1	EEE	98	4% 89% 10%
2	BBB	87	6% 80% 13% 6%
2	FFF	87	3% 84% 14%
3	CCC	107	5% 80% 19%

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Mol	Chain	Length	Quality of chain
3	GGG	107	2% 86% 14%
4	DDD	95	% 86% 14%
4	HHH	95	% 82% 16%
5	III	145	5% 68% 31%
6	JJJ	145	4% 63% 35%
7	MMM	14	50% 64% 21% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	XIS	EEE	201	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12178 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 Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	EEE	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	FFF	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	107	Total	C	N	O	0	0	0
			828	523	162	143			
3	GGG	107	Total	C	N	O	0	0	0
			828	523	162	143			

- Molecule 4 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	95	Total	C	N	O	S	0	0	0
			745	467	136	140	2			
4	HHH	95	Total	C	N	O	S	0	0	0
			745	467	136	140	2			

- Molecule 5 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	III	145	2970	1421	538	867	144	0	0	0

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	JJJ	145	2969	1421	535	869	144	0	0	0

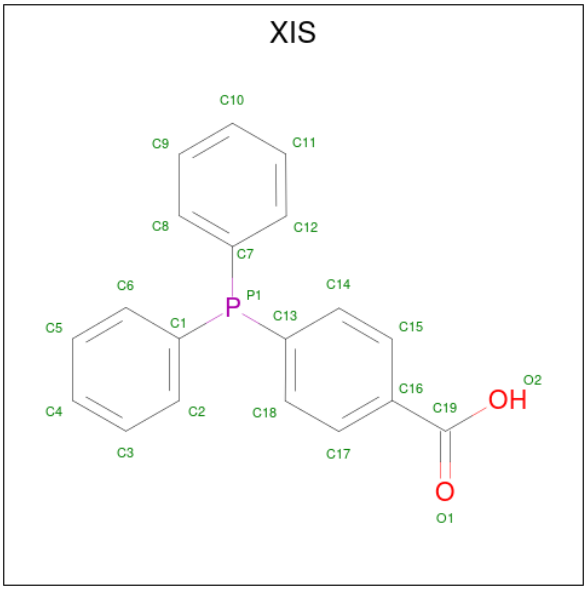
- Molecule 7 is a protein called LANA peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	MMM	14	99	58	24	17	0	0	0

- Molecule 8 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Au		
8	AAA	1	1	1	0	0

- Molecule 9 is 4-diphenylphosphanylbenzoic acid (three-letter code: XIS) (formula: $C_{19}H_{15}O_2P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
9	EEE	1	22	19	2	1	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

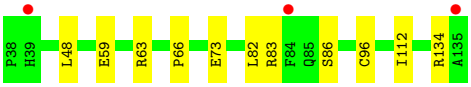
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	EEE	1	Total Mg 1 1	0	0

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.

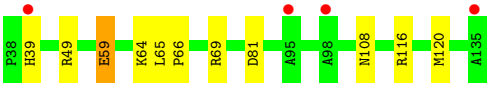
• Molecule 1: Histone H3.1

Chain AAA:



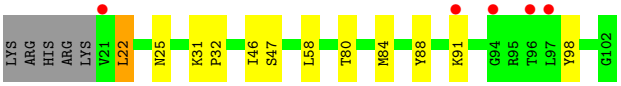
• Molecule 1: Histone H3.1

Chain EEE:



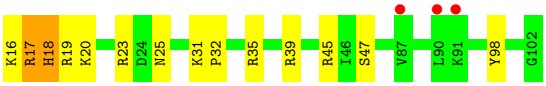
• Molecule 2: Histone H4

Chain BBB:



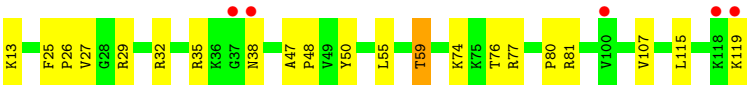
• Molecule 2: Histone H4

Chain FFF:



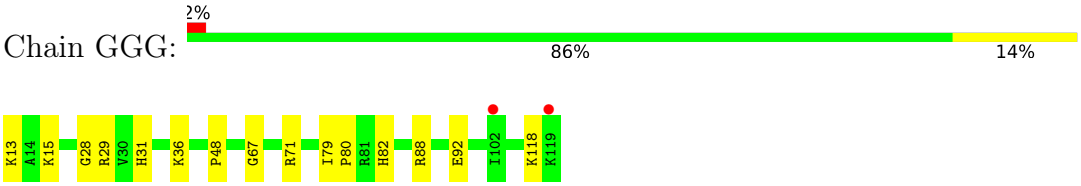
• Molecule 3: Histone H2A type 1-B/E

Chain CCC:



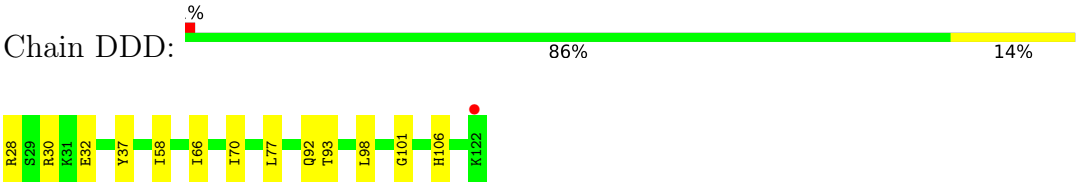
• Molecule 3: Histone H2A type 1-B/E

Chain GGG:



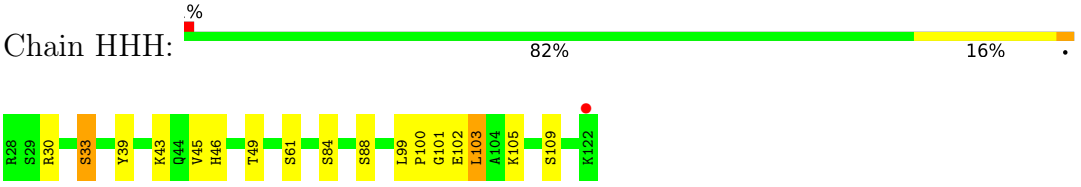
• Molecule 4: Histone H2B type 1-K

Chain DDD:



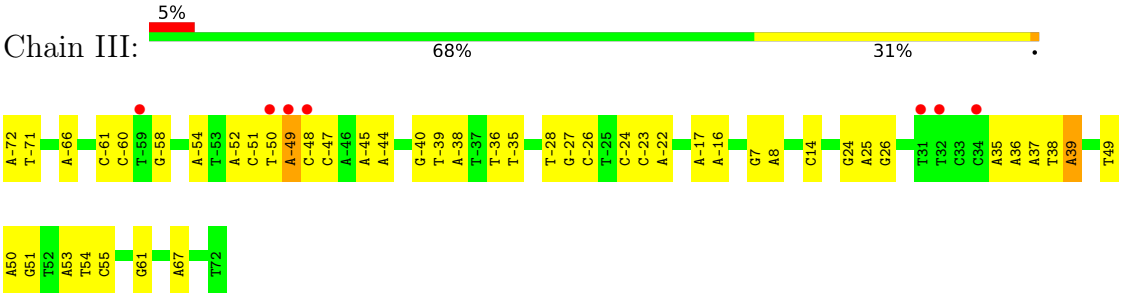
• Molecule 4: Histone H2B type 1-K

Chain HHH:



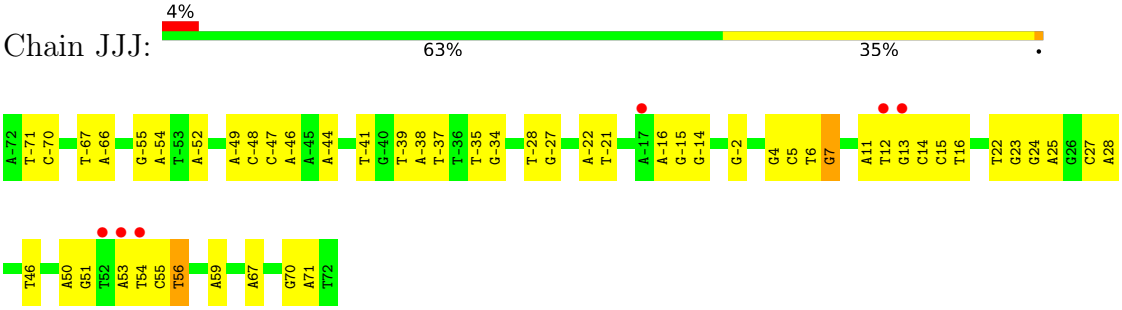
• Molecule 5: DNA (145-MER)

Chain III:



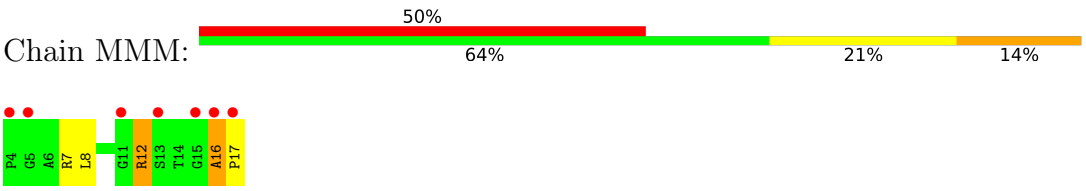
• Molecule 6: DNA (145-MER)

Chain JJJ:



• Molecule 7: LANA peptide

Chain MMM:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.11Å 109.61Å 183.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.30 48.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.93-2.30) 99.9 (48.88-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.224 , 0.262 0.226 , 0.262	Depositor DCC
R_{free} test set	1952 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12178	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ORN, AU, XIS, MG

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	AAA	0.67	0/819	0.89	1/1097 (0.1%)
1	EEE	0.75	0/819	0.94	0/1097
2	BBB	0.69	0/660	0.88	0/883
2	FFF	0.77	0/711	0.96	1/948 (0.1%)
3	CCC	0.74	0/838	0.98	0/1129
3	GGG	0.69	0/838	0.85	0/1129
4	DDD	0.74	0/756	0.84	0/1014
4	HHH	0.75	0/756	0.85	0/1014
5	III	0.48	1/3332 (0.0%)	0.89	9/5141 (0.2%)
6	JJJ	0.47	1/3330 (0.0%)	0.86	4/5138 (0.1%)
7	MMM	0.73	0/91	1.03	0/118
All	All	0.61	2/12950 (0.0%)	0.89	15/18708 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	JJJ	56	DT	O3'-P	-5.20	1.54	1.61
5	III	14	DC	O3'-P	-5.01	1.55	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	III	-49	DA	C1'-O4'-C4'	-9.22	100.88	110.10
6	JJJ	-2	DG	O5'-P-OP2	-8.00	98.50	105.70
5	III	-49	DA	N9-C1'-C2'	7.52	126.89	112.60
5	III	-40	DG	N9-C1'-C2'	6.62	125.19	112.60
6	JJJ	7	DG	O5'-P-OP1	-6.34	100.00	105.70
5	III	-49	DA	C8-N9-C1'	6.19	138.84	127.70
5	III	-49	DA	C4-N9-C1'	-6.17	115.19	126.30
5	III	8	DA	O5'-P-OP2	-5.92	100.37	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	112	ILE	C-N-CA	5.91	136.48	121.70
5	III	39	DA	O5'-P-OP1	-5.74	100.53	105.70
2	FFF	98	TYR	CB-CG-CD1	5.73	124.44	121.00
6	JJJ	7	DG	P-O5'-C5'	-5.43	112.22	120.90
5	III	-40	DG	C3'-C2'-C1'	-5.23	96.23	102.50
6	JJJ	-67	DT	C1'-O4'-C4'	-5.15	104.95	110.10
5	III	61	DG	C1'-O4'-C4'	-5.11	104.99	110.10

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	AAA	807	0	844	7	0
1	EEE	807	0	844	8	0
2	BBB	653	0	696	10	0
2	FFF	703	0	755	8	0
3	CCC	828	0	892	15	0
3	GGG	828	0	892	8	0
4	DDD	745	0	769	10	0
4	HHH	745	0	769	9	0
5	III	2970	0	1640	37	0
6	JJJ	2969	0	1641	48	0
7	MMM	99	0	104	6	0
8	AAA	1	0	0	1	0
9	EEE	22	0	0	3	0
10	EEE	1	0	0	0	0
All	All	12178	0	9846	133	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 6.

All (133) 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)
3:CCC:50:TYR:OH	4:DDD:92:GLN:NE2	2.08	0.85
6:JJJ:-49:DA:H4'	6:JJJ:-48:DC:OP1	1.79	0.83
6:JJJ:-22:DA:H2"	6:JJJ:-21:DT:O5'	1.79	0.82
1:AAA:96:CYS:SG	2:BBB:58:LEU:CD1	2.74	0.76
6:JJJ:54:DT:H2"	6:JJJ:55:DC:OP2	1.88	0.74
1:EEE:49:ARG:HH11	1:EEE:49:ARG:HG3	1.59	0.68
1:AAA:96:CYS:SG	2:BBB:58:LEU:HD13	2.33	0.67
5:III:-50:DT:C4	5:III:-49:DA:N6	2.65	0.65
5:III:53:DA:C2	6:JJJ:-52:DA:C2	2.86	0.64
7:MMM:16:ALA:CB	7:MMM:17:PRO:CD	2.77	0.63
6:JJJ:-28:DT:H3'	6:JJJ:-27:DG:H5"	1.81	0.63
5:III:-52:DA:C2	6:JJJ:53:DA:C2	2.87	0.62
8:AAA:201:AU:AU	9:EEE:201:XIS:P1	2.27	0.62
5:III:-52:DA:C2	6:JJJ:53:DA:N1	2.68	0.62
1:EEE:69:ARG:HD2	2:FFF:25:ASN:OD1	2.01	0.60
5:III:-28:DT:H4'	5:III:-27:DG:OP1	2.01	0.60
3:GGG:13:LYS:HD3	6:JJJ:-41:DT:OP1	2.01	0.60
1:AAA:73:GLU:OE1	2:BBB:25:ASN:HB2	2.01	0.59
7:MMM:16:ALA:HB3	7:MMM:17:PRO:HD2	1.85	0.59
4:HHH:45:VAL:O	7:MMM:12:ARG:NH1	2.36	0.58
5:III:-51:DC:H5"	5:III:-51:DC:H6	1.68	0.57
6:JJJ:-35:DT:H2"	6:JJJ:-34:DG:C8	2.40	0.56
6:JJJ:-28:DT:C3'	6:JJJ:-27:DG:H5"	2.36	0.56
4:DDD:77:LEU:HD21	4:DDD:93:THR:HB	1.86	0.56
2:FFF:31:LYS:N	2:FFF:32:PRO:HD2	2.21	0.56
6:JJJ:-49:DA:C4'	6:JJJ:-48:DC:OP1	2.54	0.55
3:CCC:47:ALA:HB3	3:CCC:48:PRO:HD3	1.89	0.55
3:CCC:55:LEU:O	3:CCC:59:THR:HG23	2.07	0.55
6:JJJ:13:DG:H4'	6:JJJ:14:DC:OP1	2.07	0.54
5:III:-22:DA:C2	6:JJJ:23:DG:N2	2.76	0.54
6:JJJ:11:DA:H2"	6:JJJ:12:DT:O5'	2.09	0.53
6:JJJ:14:DC:H4'	6:JJJ:15:DC:OP1	2.08	0.53
6:JJJ:50:DA:H2"	6:JJJ:51:DG:OP2	2.07	0.53
5:III:-39:DT:H2"	5:III:-38:DA:H8	1.74	0.53
2:BBB:98:TYR:CD1	4:HHH:61:SER:HB3	2.44	0.53
1:AAA:96:CYS:SG	2:BBB:58:LEU:HD11	2.48	0.53
5:III:-66:DA:C2	6:JJJ:67:DA:C2	2.97	0.53
9:EEE:201:XIS:C2	9:EEE:201:XIS:C12	2.87	0.52
5:III:-27:DG:H4'	5:III:-26:DC:OP1	2.10	0.52
3:GGG:92:GLU:HB3	4:HHH:103:LEU:HD22	1.92	0.51
1:EEE:81:ASP:HA	2:FFF:19:ARG:HH22	1.74	0.51
6:JJJ:-15:DG:H2"	6:JJJ:-14:DG:OP2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:GGG:79:ILE:HG12	3:GGG:82:HIS:CE1	2.45	0.51
3:CCC:32:ARG:HH22	4:DDD:32:GLU:CD	2.14	0.51
6:JJJ:-28:DT:H2'	6:JJJ:-27:DG:C8	2.45	0.51
5:III:-50:DT:C4	5:III:-49:DA:C6	2.99	0.50
6:JJJ:24:DG:H4'	6:JJJ:25:DA:OP1	2.11	0.49
2:FFF:17:ARG:O	2:FFF:18:HIS:O	2.29	0.49
4:DDD:28:ARG:CB	6:JJJ:50:DA:OP1	2.60	0.49
5:III:-61:DC:H2"	5:III:-60:DC:O5'	2.12	0.49
3:CCC:26:PRO:HG3	4:DDD:37:TYR:CE2	2.48	0.49
3:CCC:26:PRO:HG3	4:DDD:37:TYR:CZ	2.48	0.48
6:JJJ:53:DA:C2	6:JJJ:54:DT:C2	3.01	0.48
3:GGG:29:ARG:NH1	4:HHH:33:SER:O	2.47	0.48
5:III:-45:DA:H1'	5:III:-44:DA:H5'	1.96	0.47
6:JJJ:-47:DC:O2	6:JJJ:-46:DA:C2	2.68	0.47
3:CCC:32:ARG:NH2	4:DDD:32:GLU:OE1	2.41	0.47
7:MMM:16:ALA:HB1	7:MMM:17:PRO:HD3	1.97	0.47
3:CCC:55:LEU:O	3:CCC:59:THR:CG2	2.63	0.47
1:EEE:65:LEU:HB3	1:EEE:66:PRO:HD3	1.96	0.47
9:EEE:201:XIS:C14	9:EEE:201:XIS:C8	2.93	0.46
1:AAA:83:ARG:O	2:BBB:80:THR:HA	2.16	0.46
2:BBB:46:ILE:O	6:JJJ:7:DG:H3'	2.15	0.46
4:HHH:45:VAL:HG12	4:HHH:46:HIS:CD2	2.50	0.46
7:MMM:16:ALA:CB	7:MMM:17:PRO:HD2	2.45	0.46
7:MMM:16:ALA:HB1	7:MMM:17:PRO:CD	2.46	0.46
2:BBB:31:LYS:HB3	2:BBB:32:PRO:HD3	1.98	0.46
5:III:-17:DA:C2	5:III:-16:DA:C5	3.04	0.45
6:JJJ:-34:DG:H2'	6:JJJ:-34:DG:OP2	2.16	0.45
6:JJJ:5:DC:H4'	6:JJJ:6:DT:OP1	2.15	0.45
5:III:-51:DC:H4'	5:III:-51:DC:OP1	2.16	0.45
3:GGG:28:GLY:HA3	6:JJJ:-44:DA:H3'	1.97	0.45
5:III:-72:DA:C2	5:III:-71:DT:C2	3.04	0.45
5:III:-47:DC:N4	6:JJJ:46:DT:O4	2.50	0.45
5:III:49:DT:H2"	5:III:50:DA:C8	2.52	0.45
2:FFF:35:ARG:O	2:FFF:39:ARG:HG2	2.17	0.45
6:JJJ:-38:DA:H2"	6:JJJ:-37:DT:OP2	2.16	0.45
3:CCC:25:PHE:CZ	3:CCC:59:THR:HG21	2.52	0.44
3:CCC:80:PRO:HB3	4:DDD:58:ILE:CD1	2.48	0.44
5:III:-50:DT:O4	5:III:-49:DA:N6	2.49	0.44
2:BBB:22:LEU:HD22	2:BBB:22:LEU:C	2.37	0.44
6:JJJ:4:DG:H4'	6:JJJ:5:DC:OP1	2.17	0.44
3:CCC:32:ARG:O	3:CCC:35:ARG:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:81:ASP:HA	2:FFF:19:ARG:NH2	2.32	0.44
5:III:25:DA:H4'	5:III:26:DG:OP1	2.18	0.44
6:JJJ:22:DT:H2"	6:JJJ:23:DG:C8	2.53	0.44
5:III:39:DA:C2	6:JJJ:-38:DA:C2	3.05	0.43
5:III:-24:DC:H1'	5:III:-23:DC:C5	2.53	0.43
6:JJJ:27:DC:C4	6:JJJ:28:DA:C6	3.06	0.43
6:JJJ:50:DA:C6	6:JJJ:51:DG:C6	3.07	0.43
5:III:24:DG:H2"	5:III:25:DA:OP2	2.18	0.43
6:JJJ:-71:DT:H2"	6:JJJ:-70:DC:O5'	2.18	0.43
6:JJJ:11:DA:C2'	6:JJJ:12:DT:O5'	2.66	0.43
5:III:35:DA:H4'	5:III:36:DA:OP1	2.19	0.43
6:JJJ:-55:DG:H2"	6:JJJ:-54:DA:OP2	2.19	0.43
3:GGG:31:HIS:CD2	3:GGG:48:PRO:HG3	2.54	0.43
6:JJJ:15:DC:H2"	6:JJJ:16:DT:OP2	2.18	0.43
4:DDD:66:ILE:HG22	4:DDD:70:ILE:HD12	2.01	0.42
5:III:-39:DT:H2"	5:III:-38:DA:C8	2.53	0.42
1:EEE:59:GLU:H	1:EEE:59:GLU:HG3	1.63	0.42
4:HHH:46:HIS:HB3	4:HHH:49:THR:HB	2.01	0.42
5:III:54:DT:H2"	5:III:55:DC:C6	2.54	0.42
5:III:-50:DT:H5'	5:III:-49:DA:OP2	2.19	0.42
3:CCC:81:ARG:NH2	3:CCC:107:VAL:O	2.38	0.42
1:EEE:116:ARG:NH1	1:EEE:120:MET:HG3	2.35	0.42
6:JJJ:55:DC:H6	6:JJJ:55:DC:O5'	2.03	0.42
6:JJJ:70:DG:H2"	6:JJJ:71:DA:OP2	2.19	0.42
5:III:-24:DC:H1'	5:III:-23:DC:C6	2.55	0.41
3:CCC:77:ARG:HD3	5:III:-54:DA:H5"	2.02	0.41
3:GGG:67:GLY:HA3	4:HHH:46:HIS:CD2	2.55	0.41
3:GGG:79:ILE:HB	3:GGG:80:PRO:HD2	2.00	0.41
5:III:37:DA:H2"	5:III:38:DT:OP2	2.21	0.41
2:FFF:45:ARG:CZ	5:III:7:DG:H4'	2.49	0.41
5:III:-58:DG:N2	6:JJJ:59:DA:C2	2.89	0.41
6:JJJ:55:DC:C2'	6:JJJ:56:DT:O5'	2.68	0.41
4:HHH:39:TYR:CE1	4:HHH:43:LYS:HE2	2.55	0.41
2:BBB:84:MET:HE2	2:BBB:88:TYR:CZ	2.56	0.41
5:III:67:DA:C2	6:JJJ:-66:DA:C2	3.09	0.41
6:JJJ:-16:DA:H4'	6:JJJ:-15:DG:OP1	2.20	0.41
1:AAA:63:ARG:HB2	1:AAA:66:PRO:HG2	2.02	0.41
3:CCC:27:VAL:HG13	3:CCC:48:PRO:HB2	2.03	0.41
2:FFF:31:LYS:N	2:FFF:32:PRO:CD	2.83	0.41
5:III:-49:DA:C6	5:III:-48:DC:N3	2.89	0.41
5:III:-36:DT:C2	5:III:-35:DT:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:III:50:DA:H2"	5:III:51:DG:O4'	2.21	0.41
6:JJJ:-15:DG:C2'	6:JJJ:-14:DG:OP2	2.69	0.41
4:HHH:99:LEU:HA	4:HHH:100:PRO:HD3	1.91	0.41
1:AAA:82:LEU:HD23	1:AAA:82:LEU:HA	1.86	0.40
4:DDD:28:ARG:HB2	6:JJJ:50:DA:OP1	2.21	0.40
6:JJJ:-39:DT:H2"	6:JJJ:-38:DA:H8	1.86	0.40
6:JJJ:55:DC:C6	6:JJJ:56:DT:H72	2.56	0.40
5:III:-51:DC:H5"	5:III:-51:DC:C6	2.53	0.40
3:CCC:115:LEU:HD11	1:EEE:108:ASN:HD21	1.86	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	AAA	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
1	EEE	96/98 (98%)	96 (100%)	0	0	100	100
2	BBB	80/87 (92%)	80 (100%)	0	0	100	100
2	FFF	85/87 (98%)	82 (96%)	2 (2%)	1 (1%)	13	14
3	CCC	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	GGG	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
4	DDD	93/95 (98%)	85 (91%)	7 (8%)	1 (1%)	14	15
4	HHH	93/95 (98%)	91 (98%)	1 (1%)	1 (1%)	14	15
7	MMM	11/14 (79%)	8 (73%)	2 (18%)	1 (9%)	1	0
All	All	764/788 (97%)	734 (96%)	26 (3%)	4 (0%)	29	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	FFF	18	HIS
7	MMM	16	ALA
4	DDD	101	GLY
4	HHH	101	GLY

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	AAA	85/85 (100%)	81 (95%)	4 (5%)	26	37
1	EEE	85/85 (100%)	82 (96%)	3 (4%)	36	50
2	BBB	67/72 (93%)	64 (96%)	3 (4%)	27	39
2	FFF	72/72 (100%)	67 (93%)	5 (7%)	15	20
3	CCC	85/85 (100%)	78 (92%)	7 (8%)	11	14
3	GGG	85/85 (100%)	80 (94%)	5 (6%)	19	27
4	DDD	81/81 (100%)	78 (96%)	3 (4%)	34	48
4	HHH	81/81 (100%)	73 (90%)	8 (10%)	8	9
7	MMM	9/9 (100%)	6 (67%)	3 (33%)	0	0
All	All	650/655 (99%)	609 (94%)	41 (6%)	18	24

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	48	LEU
1	AAA	59	GLU
1	AAA	86	SER
1	AAA	134	ARG
2	BBB	22	LEU
2	BBB	47	SER
2	BBB	91	LYS
3	CCC	13	LYS
3	CCC	29	ARG
3	CCC	38	ASN
3	CCC	59	THR

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Mol	Chain	Res	Type
3	CCC	74	LYS
3	CCC	76	THR
3	CCC	119	LYS
4	DDD	30	ARG
4	DDD	98	LEU
4	DDD	106	HIS
1	EEE	39	HIS
1	EEE	59	GLU
1	EEE	64	LYS
2	FFF	16	LYS
2	FFF	17	ARG
2	FFF	20	LYS
2	FFF	23	ARG
2	FFF	47	SER
3	GGG	15	LYS
3	GGG	36	LYS
3	GGG	71	ARG
3	GGG	88	ARG
3	GGG	118	LYS
4	HHH	30	ARG
4	HHH	33	SER
4	HHH	84	SER
4	HHH	88	SER
4	HHH	102	GLU
4	HHH	103	LEU
4	HHH	105	LYS
4	HHH	109	SER
7	MMM	7	ARG
7	MMM	8	LEU
7	MMM	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ORN	MMM	6	7	6,7,8	0.50	0	2,7,9	0.36	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
7	ORN	MMM	6	7	-	1/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	MMM	6	ORN	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
9	XIS	EEE	201	-	24,24,24	0.67	0	32,32,32	1.73	6 (18%)

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
9	XIS	EEE	201	-	-	3/16/16/16	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	EEE	201	XIS	C7-P1-C1	-4.86	94.16	102.40
9	EEE	201	XIS	C13-P1-C1	4.75	110.46	102.40
9	EEE	201	XIS	C13-P1-C7	4.48	109.99	102.40
9	EEE	201	XIS	C17-C16-C15	2.59	122.27	118.59
9	EEE	201	XIS	C15-C14-C13	-2.05	119.36	121.27
9	EEE	201	XIS	C18-C17-C16	-2.01	118.44	120.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	EEE	201	XIS	C2-C1-P1-C7
9	EEE	201	XIS	C18-C13-P1-C1
9	EEE	201	XIS	C6-C1-P1-C7

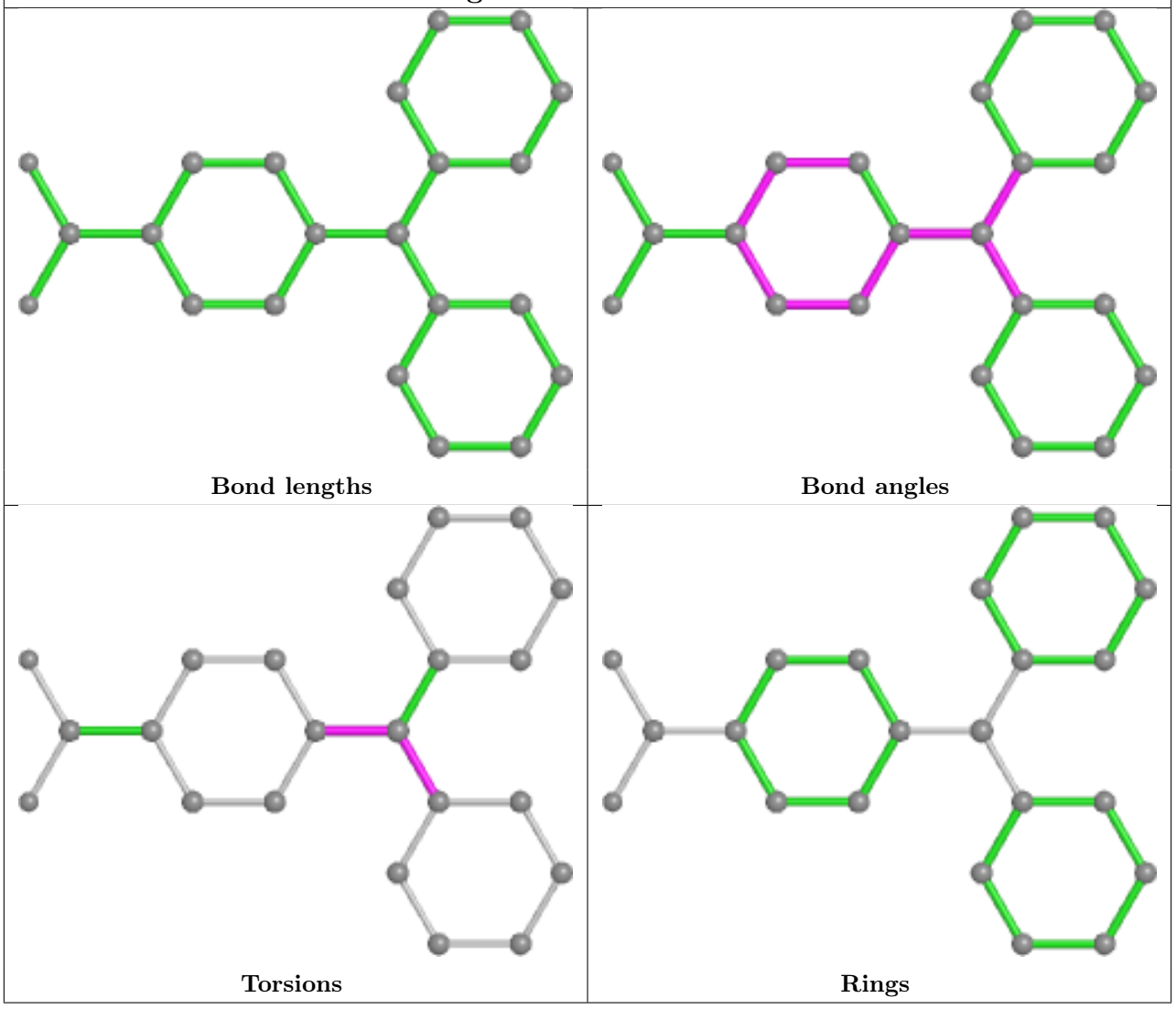
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	EEE	201	XIS	3	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand XIS EEE 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	AAA	98/98 (100%)	0.41	3 (3%)	49	56	48, 72, 112, 164	0
1	EEE	98/98 (100%)	0.44	4 (4%)	37	44	40, 57, 89, 137	0
2	BBB	82/87 (94%)	0.44	5 (6%)	21	27	54, 69, 94, 169	0
2	FFF	87/87 (100%)	0.61	3 (3%)	45	52	45, 56, 88, 165	0
3	CCC	107/107 (100%)	0.35	5 (4%)	31	38	44, 65, 114, 151	0
3	GGG	107/107 (100%)	0.36	2 (1%)	66	73	52, 73, 118, 171	0
4	DDD	95/95 (100%)	0.36	1 (1%)	80	85	49, 71, 119, 163	0
4	HHH	95/95 (100%)	0.44	1 (1%)	80	85	55, 74, 128, 170	0
5	III	145/145 (100%)	0.02	7 (4%)	30	37	72, 129, 174, 242	0
6	JJJ	145/145 (100%)	0.02	6 (4%)	37	44	73, 127, 180, 237	0
7	MMM	13/14 (92%)	4.24	7 (53%)	0	0	101, 181, 225, 251	0
All	All	1072/1078 (99%)	0.36	44 (4%)	37	44	40, 76, 163, 251	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	MMM	17	PRO	15.2
7	MMM	16	ALA	13.7
7	MMM	4	PRO	6.6
3	GGG	119	LYS	5.3
3	CCC	119	LYS	5.2
1	AAA	135	ALA	5.2
6	JJJ	13	DG	5.2
5	III	32	DT	4.5
7	MMM	15	GLY	4.5
7	MMM	5	GLY	3.7
7	MMM	11	GLY	3.5
1	AAA	84	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
4	DDD	122	LYS	3.1
6	JJJ	12	DT	3.1
5	III	31	DT	3.1
3	CCC	37	GLY	2.9
2	BBB	97	LEU	2.8
2	FFF	91	LYS	2.8
6	JJJ	53	DA	2.8
1	EEE	135	ALA	2.8
1	EEE	39	HIS	2.8
3	CCC	38	ASN	2.7
6	JJJ	-17	DA	2.7
1	AAA	39	HIS	2.6
6	JJJ	52	DT	2.5
5	III	34	DC	2.5
4	HHH	122	LYS	2.5
2	BBB	94	GLY	2.5
6	JJJ	54	DT	2.5
2	FFF	90	LEU	2.5
3	GGG	102	ILE	2.5
1	EEE	95	ALA	2.4
2	BBB	96	THR	2.4
2	BBB	21	VAL	2.4
3	CCC	118	LYS	2.4
5	III	-48	DC	2.3
2	FFF	87	VAL	2.3
7	MMM	13	SER	2.3
2	BBB	91	LYS	2.1
1	EEE	98	ALA	2.1
5	III	-50	DT	2.1
3	CCC	100	VAL	2.1
5	III	-49	DA	2.1
5	III	-59	DT	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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
7	ORN	MMM	6	8/9	0.77	0.32	131,148,155,161	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

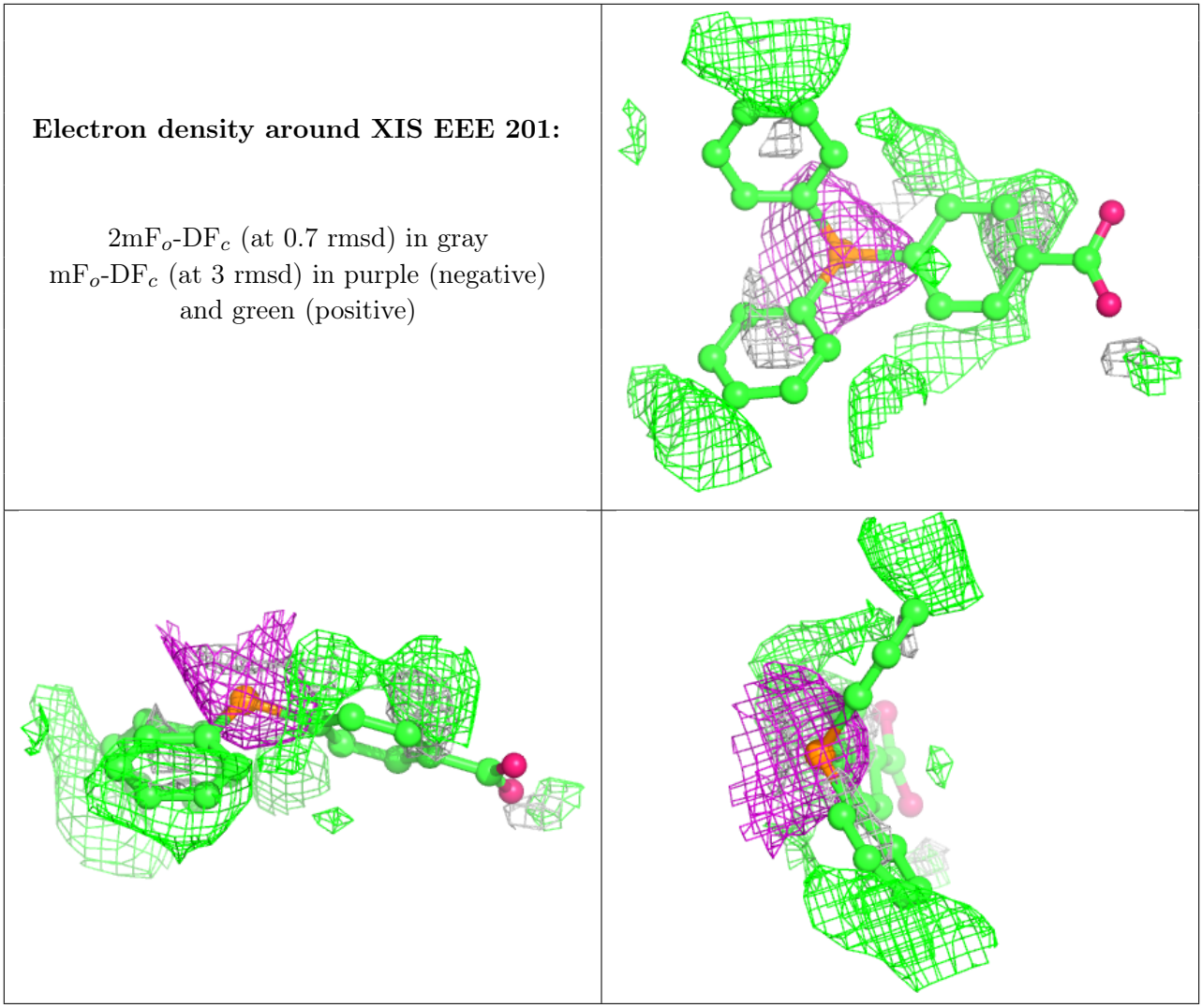
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
9	XIS	EEE	201	22/22	0.04	1.11	114,122,150,154	22
8	AU	AAA	201	1/1	0.84	0.30	135,135,135,135	1
10	MG	EEE	202	1/1	0.95	0.36	53,53,53,53	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 XIS EEE 201:

$2mF_o$-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.