



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:29 am BST

PDB ID : 2V8X
Title : Crystallographic and mass spectrometric characterisation of eIF4E with N7-cap derivatives
Authors : Brown, C.J.; Mcnae, I.; Fischer, P.M.; Walkinshaw, M.D.
Deposited on : 2007-08-16
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 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 : 2.11
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) : 2.11

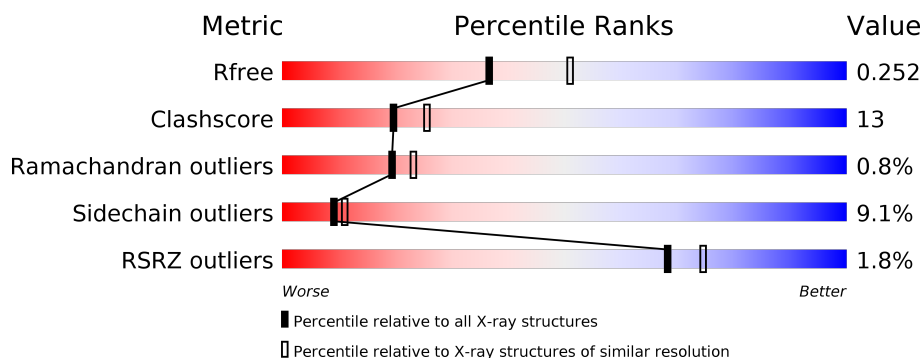
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 on 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	217	
1	E	217	
2	B	14	
2	F	14	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3651 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.

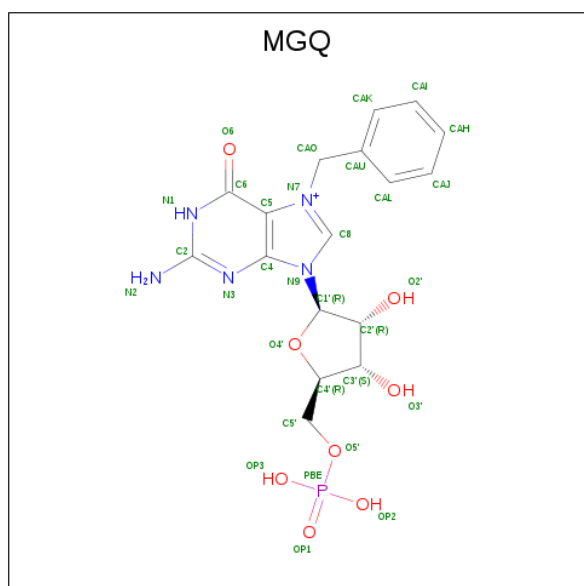
- Molecule 1 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1504	960	265	273	6			
1	E	179	Total	C	N	O	S	0	0	0
			1484	948	261	269	6			

- Molecule 2 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 4E-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			129	81	25	21	2			
2	F	14	Total	C	N	O	S	0	0	0
			129	81	25	21	2			

- Molecule 3 is 7-BENZYL GUANINE MONOPHOSPHATE (three-letter code: MGQ) (formula: $C_{17}H_{21}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	5	8	1		
3	E	1	Total	C	N	O	P	0	0
			31	17	5	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	18	Total	O	0	0
			18	18		
4	E	146	Total	O	0	0
			146	146		
4	F	22	Total	O	0	0
			22	22		

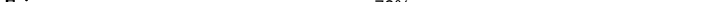
- Molecule 1: EUKARYOTIC TRANSLATION INITIATION FACTOR 4E

NET	ALA	THR	VAL	GLU	PRO	GLU	THR	PRO	THR	PRO	ASN	PRO	THR	THR	GLU	GLU	GLU	LYS	GLU	SER	ASN	GLN	GLU	VAL	ALA	ASN	PRO	E32	H33	Y34	I35	L45	F48	Q57	R61	L62	I63	S64	K65	A74	C89	D90	Y91	E99	P100	M101	M102	F106
	K108		H112	R113	L114	M118	Q121	D125	R128	L134	L137	I138	D148	V149	V153	V154	K159	H166	E169	C170	E171	M172	R173	T177	R186	K192	I195	G196	Y197	Q198	S199	T205	LVS	SER	GLY	SER	THR	T211	K212	F215	V216	H117						

Chain E: 

R186	E70	E77	E83	E86	D96	M101	R112	Q120	L135	D143	D148	V156	K159	A164	E169	H178	G180	R181	K184	V194	R192	R193	R194	R195	R196	R197	R198	R199	R200	R201	R202	R203	R204	R205	R206	R207	R208	R209	R210	R211	R212	R213	R214	R215	R216	R217	R218	R219	R220	R221	R222	R223	R224	R225	R226	R227	R228	R229	R230	R231	R232	R233	R234	R235	R236	R237	R238	R239	R240	R241	R242	R243	R244	R245	R246	R247	R248	R249	R250	R251	R252	R253	R254	R255	R256	R257	R258	R259	R260	R261	R262	R263	R264	R265	R266	R267	R268	R269	R270	R271	R272	R273	R274	R275	R276	R277	R278	R279	R280	R281	R282	R283	R284	R285	R286	R287	R288	R289	R290	R291	R292	R293	R294	R295	R296	R297	R298	R299	R300	R301	R302	R303	R304	R305	R306	R307	R308	R309	R310	R311	R312	R313	R314	R315	R316	R317	R318	R319	R320	R321	R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682</
------	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	--------

Chain B: 86% 7% 7%

Chain F:  7% 79% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.26Å 100.21Å 135.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.10 – 2.30 40.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (41.10-2.30) 90.0 (40.26-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.259 0.184 , 0.252	Depositor DCC
R_{free} test set	1117 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3651	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MGQ

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	0.83	1/1542 (0.1%)	0.86	1/2084 (0.0%)
1	E	0.88	1/1521 (0.1%)	0.89	5/2055 (0.2%)
2	B	0.79	0/130	0.84	0/169
2	F	0.82	0/130	0.77	0/169
All	All	0.85	2/3323 (0.1%)	0.87	6/4477 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	185	GLU	CG-CD	5.69	1.60	1.51
1	A	74	ALA	CA-CB	5.64	1.64	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	E	42	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	E	62	LEU	CA-CB-CG	5.75	128.52	115.30
1	E	114	LEU	CA-CB-CG	5.75	128.51	115.30
1	E	42	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	E	60	LEU	CA-CB-CG	5.30	127.48	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	202	ASP	Peptide

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	1504	0	1468	33	0
1	E	1484	0	1451	48	1
2	B	129	0	132	1	0
2	F	129	0	132	2	0
3	A	31	0	19	1	0
3	E	31	0	19	1	0
4	A	157	0	0	11	0
4	B	18	0	0	1	0
4	E	146	0	0	23	1
4	F	22	0	0	1	0
All	All	3651	0	3221	83	2

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 13.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:HG2	4:A:2090:HOH:O	1.47	1.15
1:A:159:LYS:HG2	4:A:2110:HOH:O	1.58	1.02
1:E:37:HIS:HD2	1:E:70:GLU:OE1	1.49	0.95
1:A:173:ARG:O	1:A:177:THR:HB	1.70	0.89
1:E:186:ARG:NH2	4:E:2125:HOH:O	2.10	0.85
1:E:49:LYS:HG2	4:E:2009:HOH:O	1.76	0.84
1:A:172:ASN:HB3	4:A:2119:HOH:O	1.85	0.76
1:A:61:ARG:NH1	4:A:2026:HOH:O	2.20	0.74
1:E:47:PHE:HB2	1:E:63:ILE:HD11	1.70	0.73
1:A:195:ILE:HD11	4:A:2123:HOH:O	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:HIS:HB2	4:E:2034:HOH:O	1.87	0.72
1:E:37:HIS:CD2	1:E:70:GLU:OE1	2.39	0.70
1:E:137:LEU:HD22	1:E:149:VAL:HG11	1.77	0.66
1:E:74:ALA:O	1:E:78:HIS:CD2	2.51	0.64
1:E:103:GLU:HG3	4:E:2059:HOH:O	1.97	0.64
1:E:113:TRP:O	1:E:164:ALA:HA	2.00	0.61
1:E:202:ASP:OD1	1:E:203:THR:N	2.31	0.60
1:A:137:LEU:HD22	1:A:149:VAL:HG11	1.83	0.58
1:E:159:LYS:H	1:E:159:LYS:HD3	1.67	0.58
1:E:200:HIS:HE1	4:E:2066:HOH:O	1.86	0.58
1:E:120:GLN:NE2	4:E:2076:HOH:O	2.38	0.57
1:A:195:ILE:CD1	4:A:2123:HOH:O	2.50	0.56
1:E:120:GLN:HE22	1:E:125:ASP:H	1.54	0.55
1:E:159:LYS:NZ	4:E:2105:HOH:O	2.29	0.55
1:A:105:GLU:OE1	1:A:108:LYS:NZ	2.40	0.54
1:E:56:TRP:HZ3	1:E:101:MET:HE2	1.72	0.54
1:A:128:ARG:CG	4:A:2090:HOH:O	2.25	0.54
1:A:125:ASP:OD2	1:A:128:ARG:NH2	2.35	0.54
1:A:118:ASN:H	1:A:121:GLN:HE21	1.55	0.53
1:E:210:THR:HG21	4:E:2136:HOH:O	2.07	0.53
1:E:42:ARG:NE	4:E:2006:HOH:O	2.20	0.53
1:E:191:PRO:HA	4:E:2123:HOH:O	2.09	0.53
1:A:118:ASN:ND2	1:A:121:GLN:HG3	2.23	0.53
1:A:32:GLU:N	4:A:2004:HOH:O	2.42	0.52
1:E:190:PRO:HG2	1:E:193:ILE:HB	1.91	0.52
1:E:86:MET:CE	4:E:2043:HOH:O	2.58	0.52
2:F:51:ARG:HD3	4:F:2002:HOH:O	2.09	0.52
1:A:166:TRP:CH2	3:A:1218:MGQ:HAK	2.45	0.52
1:A:173:ARG:O	1:A:177:THR:CB	2.54	0.51
1:E:112:ARG:HG2	1:E:112:ARG:O	2.11	0.50
1:E:58:ALA:HB1	4:E:2017:HOH:O	2.11	0.50
1:A:192:LYS:HD2	4:A:2131:HOH:O	2.13	0.49
4:E:2124:HOH:O	2:F:56:ARG:HG3	2.12	0.49
2:B:55:ASP:HB2	4:B:2008:HOH:O	2.11	0.49
1:E:184:LYS:HE2	4:E:2129:HOH:O	2.12	0.49
1:A:134:LEU:O	1:A:138:ILE:HG12	2.13	0.49
1:A:62:LEU:HD21	1:A:65:LYS:HE3	1.95	0.49
1:E:132:GLU:OE2	1:E:186:ARG:NH1	2.45	0.48
1:A:169:GLU:OE1	1:A:171:GLU:HG2	2.14	0.48
1:E:186:ARG:NH1	4:E:2124:HOH:O	2.44	0.47
1:A:61:ARG:HG3	4:A:2022:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:GLU:OE1	1:E:171:GLU:HG2	2.15	0.47
1:A:171:GLU:OE1	1:A:171:GLU:HA	2.15	0.47
1:A:177:THR:CG2	1:E:143:ASP:HB3	2.46	0.46
1:E:102:TRP:HE3	3:E:1218:MGQ:CAK	2.28	0.46
1:A:61:ARG:HB3	1:A:61:ARG:NH1	2.30	0.46
1:E:212:LYS:HE3	4:E:2137:HOH:O	2.14	0.46
1:E:200:HIS:C	1:E:202:ASP:H	2.18	0.46
1:E:135:LEU:HB2	4:E:2124:HOH:O	2.15	0.46
1:E:48:PHE:CE1	1:E:59:ASN:HB2	2.51	0.45
1:A:118:ASN:HD21	1:A:121:GLN:HG3	1.81	0.45
1:E:49:LYS:CG	4:E:2009:HOH:O	2.49	0.44
1:A:91:TYR:HB2	1:A:154:VAL:CG1	2.48	0.44
1:A:112:ARG:O	1:A:197:TYR:HA	2.17	0.44
1:A:34:TYR:CE2	1:A:35:ILE:HG13	2.52	0.44
1:E:65:LYS:NZ	1:E:96:ASP:OD1	2.33	0.44
1:E:86:MET:HE2	4:E:2043:HOH:O	2.18	0.43
1:A:173:ARG:HG3	1:A:215:PHE:CE2	2.53	0.43
1:E:43:TRP:CH2	1:E:137:LEU:HB3	2.53	0.43
1:E:145:TYR:O	1:E:179:ILE:HD11	2.19	0.43
1:E:209:SER:O	1:E:210:THR:HG22	2.19	0.43
1:E:190:PRO:HA	1:E:191:PRO:HD2	1.89	0.42
1:A:57:GLN:HG2	1:A:101:MET:CE	2.49	0.42
1:E:78:HIS:CE1	4:E:2035:HOH:O	2.72	0.42
1:E:54:LYS:HB3	1:E:58:ALA:HB3	2.01	0.42
1:A:45:LEU:HD23	1:A:63:ILE:HD12	2.02	0.41
4:A:2151:HOH:O	1:E:178:HIS:HD2	2.02	0.41
1:E:46:TRP:CZ2	1:E:62:LEU:HD22	2.54	0.41
1:E:184:LYS:HE2	1:E:217:VAL:O	2.20	0.41
1:A:177:THR:HG22	4:E:2094:HOH:O	2.20	0.41
1:E:181:ARG:NH2	4:E:2121:HOH:O	2.52	0.41
1:E:181:ARG:NE	4:E:2121:HOH:O	2.05	0.41
1:A:48:PHE:O	1:A:89:CYS:HA	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2002:HOH:O	4:E:2052:HOH:O[1_655]	2.07	0.13
1:E:78:HIS:CD2	1:E:83:SER:O[4_556]	2.16	0.04

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	177/217 (82%)	171 (97%)	6 (3%)	0	100	100
1	E	175/217 (81%)	165 (94%)	7 (4%)	3 (2%)	9	8
2	B	12/14 (86%)	12 (100%)	0	0	100	100
2	F	12/14 (86%)	12 (100%)	0	0	100	100
All	All	376/462 (81%)	360 (96%)	13 (4%)	3 (1%)	19	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	210	THR
1	E	201	ALA
1	E	194	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/195 (83%)	151 (93%)	11 (7%)	16	21
1	E	160/195 (82%)	142 (89%)	18 (11%)	6	6
2	B	14/14 (100%)	12 (86%)	2 (14%)	3	3
2	F	14/14 (100%)	13 (93%)	1 (7%)	14	19
All	All	350/418 (84%)	318 (91%)	32 (9%)	9	11

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	A	102	TRP
1	A	114	LEU
1	A	118	ASN
1	A	148	ASP
1	A	153	VAL
1	A	192	LYS
1	A	199	SER
1	A	211	THR
1	A	212	LYS
1	A	216	VAL
2	B	55	ASP
2	B	57	LYS
1	E	62	LEU
1	E	64	SER
1	E	102	TRP
1	E	112	ARG
1	E	114	LEU
1	E	117	LEU
1	E	122	ARG
1	E	124	SER
1	E	148	ASP
1	E	156	VAL
1	E	159	LYS
1	E	185	GLU
1	E	186	ARG
1	E	198	GLN
1	E	203	THR
1	E	210	THR
1	E	211	THR
1	E	212	LYS
2	F	57	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	118	ASN
1	A	121	GLN
1	E	37	HIS
1	E	120	GLN
1	E	178	HIS
1	E	198	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	200	HIS
1	E	213	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	$\# Z > 2$
3	MGQ	A	1218	-	31,34,34	1.33	3 (9%)	36,51,51	1.90	9 (25%)
3	MGQ	E	1218	-	31,34,34	1.52	4 (12%)	36,51,51	1.66	7 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGQ	A	1218	-	-	3/10/30/30	0/4/4/4
3	MGQ	E	1218	-	-	0/10/30/30	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1218	MGQ	C6-N1	4.81	1.41	1.33
3	A	1218	MGQ	C6-N1	4.46	1.40	1.33
3	E	1218	MGQ	C2-N1	4.12	1.42	1.35
3	E	1218	MGQ	O4'-C1'	3.78	1.46	1.41
3	A	1218	MGQ	C2-N1	2.79	1.40	1.35
3	A	1218	MGQ	PBE-OP3	2.47	1.64	1.54
3	E	1218	MGQ	PBE-OP2	2.02	1.62	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1218	MGQ	N3-C2-N1	-4.71	120.94	127.22
3	E	1218	MGQ	C5-C6-N1	-4.48	117.30	123.43
3	A	1218	MGQ	C5-C6-N1	-4.39	117.42	123.43
3	E	1218	MGQ	N3-C2-N1	-4.26	121.55	127.22
3	A	1218	MGQ	C2-N3-C4	3.99	119.92	115.36
3	A	1218	MGQ	O5'-PBE-OP1	3.85	117.28	106.47
3	E	1218	MGQ	C2-N3-C4	3.73	119.62	115.36
3	A	1218	MGQ	CAO-N7-C8	-3.21	121.88	125.66
3	A	1218	MGQ	O4'-C4'-C5'	-3.00	99.51	109.37
3	E	1218	MGQ	O5'-PBE-OP1	2.95	114.75	106.47
3	A	1218	MGQ	C6-N1-C2	2.93	120.58	115.93
3	E	1218	MGQ	C1'-N9-C4	-2.51	122.24	126.64
3	E	1218	MGQ	C6-N1-C2	2.45	119.82	115.93
3	A	1218	MGQ	PBE-O5'-C5'	2.15	124.21	118.30
3	A	1218	MGQ	C6-C5-C4	-2.07	118.82	120.80
3	E	1218	MGQ	N2-C2-N1	2.03	120.41	117.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

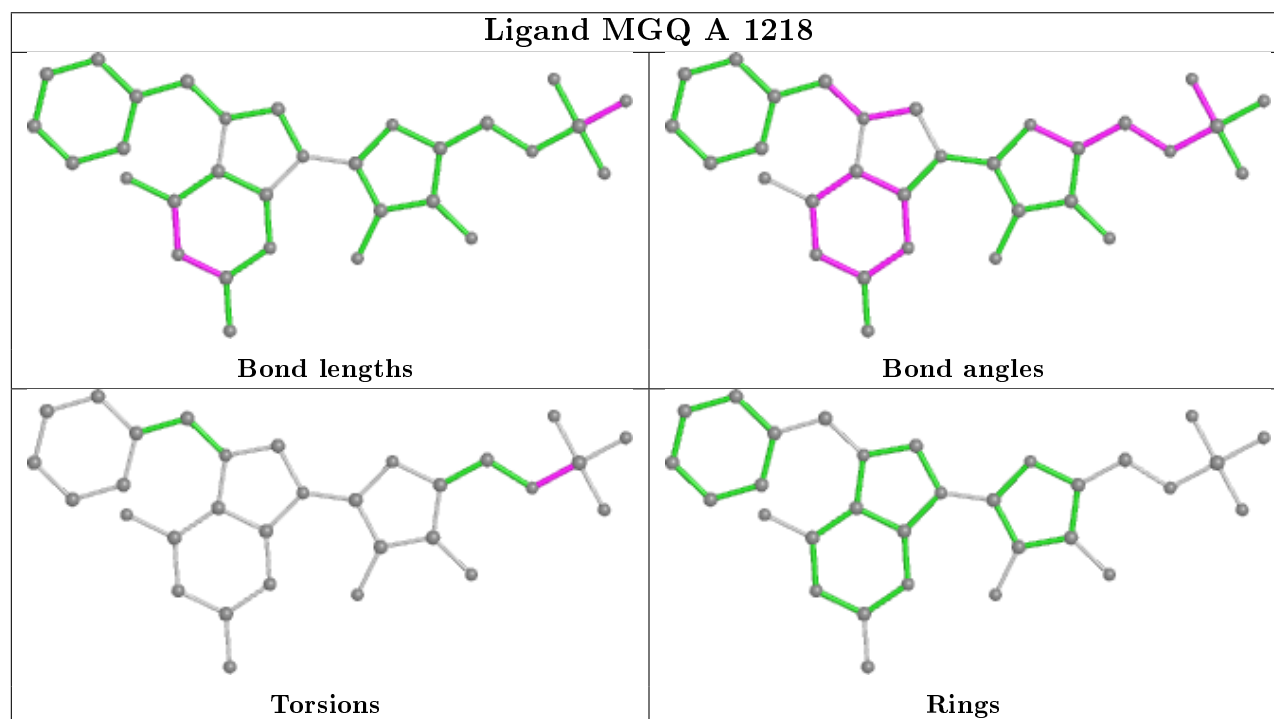
Mol	Chain	Res	Type	Atoms
3	A	1218	MGQ	C5'-O5'-PBE-OP2
3	A	1218	MGQ	C5'-O5'-PBE-OP3
3	A	1218	MGQ	C5'-O5'-PBE-OP1

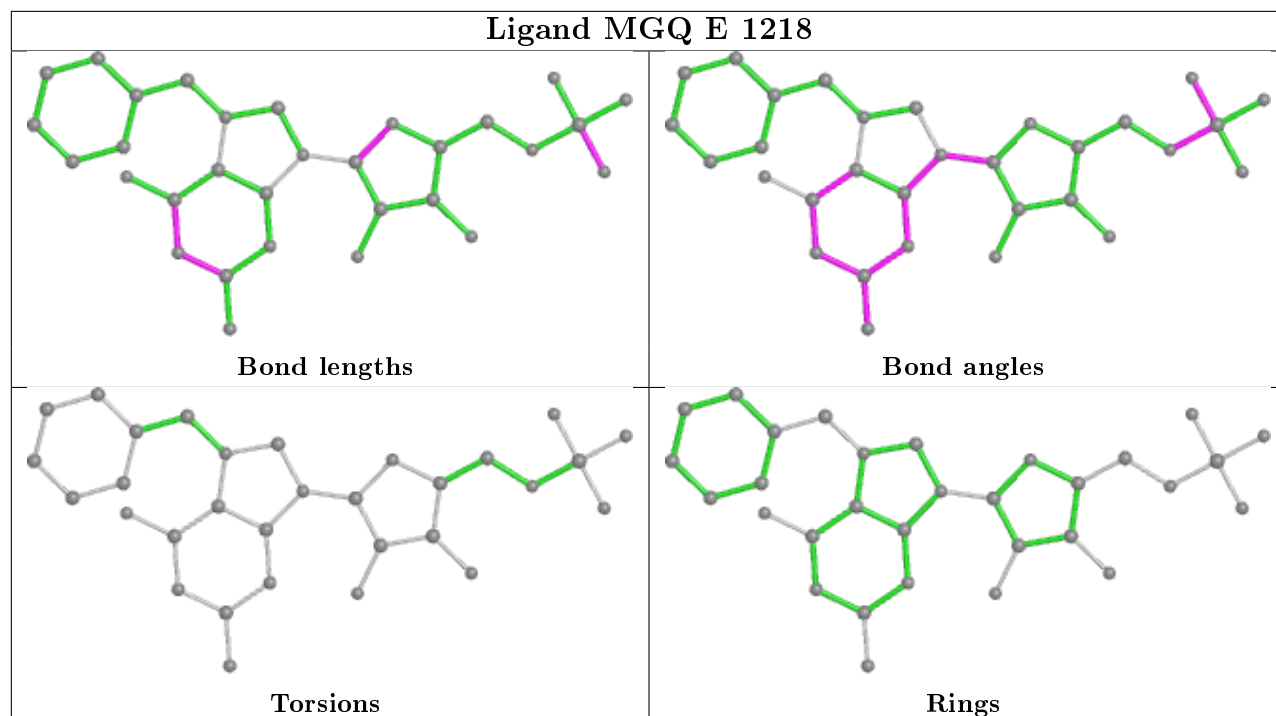
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1218	MGQ	1	0
3	E	1218	MGQ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	181/217 (83%)	-0.46	0 100 100	7, 18, 29, 37	0
1	E	179/217 (82%)	-0.19	6 (3%) 45 52	7, 16, 42, 49	0
2	B	14/14 (100%)	0.19	0 100 100	20, 32, 43, 44	0
2	F	14/14 (100%)	-0.19	1 (7%) 16 21	15, 20, 32, 33	0
All	All	388/462 (83%)	-0.30	7 (1%) 68 74	7, 18, 37, 49	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	53	SER	5.3
1	E	52	LYS	4.0
1	E	55	THR	3.3
1	E	212	LYS	2.8
1	E	51	ASP	2.2
2	F	64	ASN	2.0
1	E	191	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

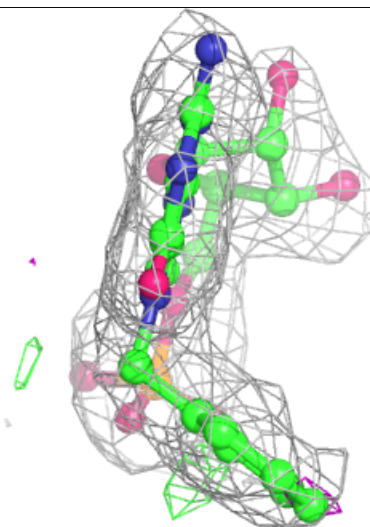
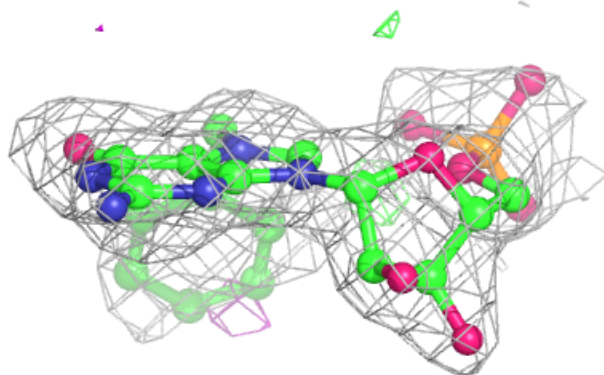
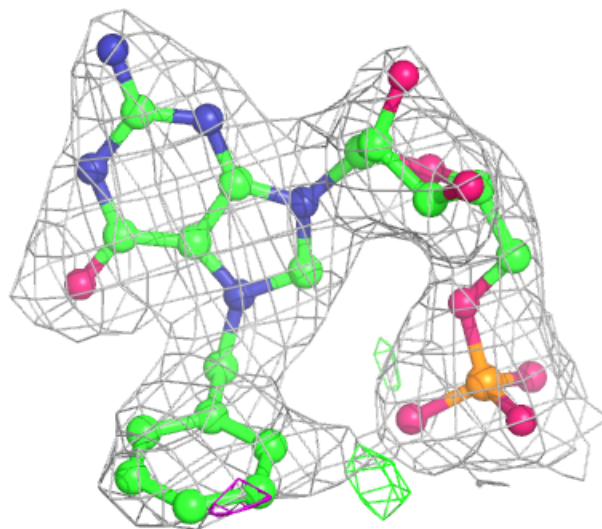
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MGQ	E	1218	31/31	0.94	0.13	32,38,48,49	0
3	MGQ	A	1218	31/31	0.97	0.10	14,16,25,27	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.

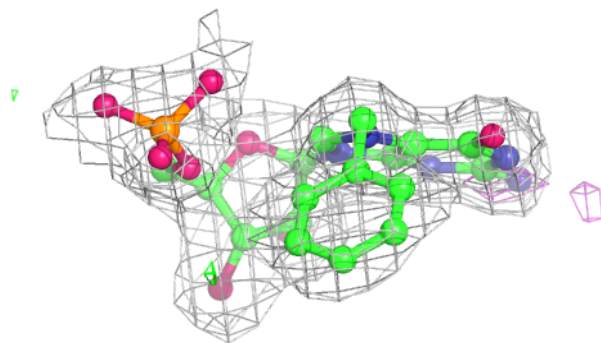
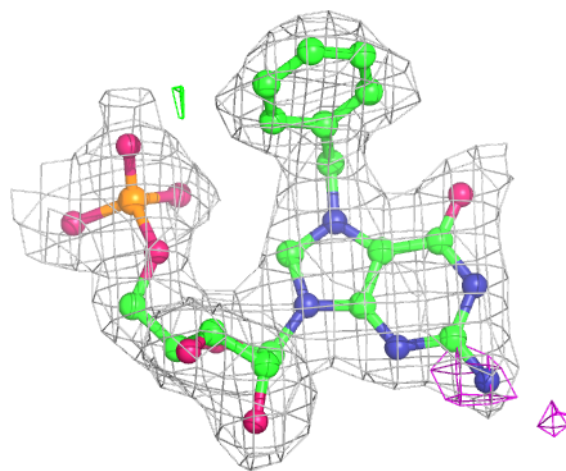
Electron density around MGQ E 1218:

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 MGQ A 1218:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.