



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2021 – 10:08 AM JST

PDB ID : 7E6G
Title : Crystal structure of diguanylate cyclase SiaD in complex with its activator SiaC from *Pseudomonas aeruginosa*
Authors : Zhou, J.S.; Zhang, L.; Zhang, L.
Deposited on : 2021-02-22
Resolution : 2.65 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:

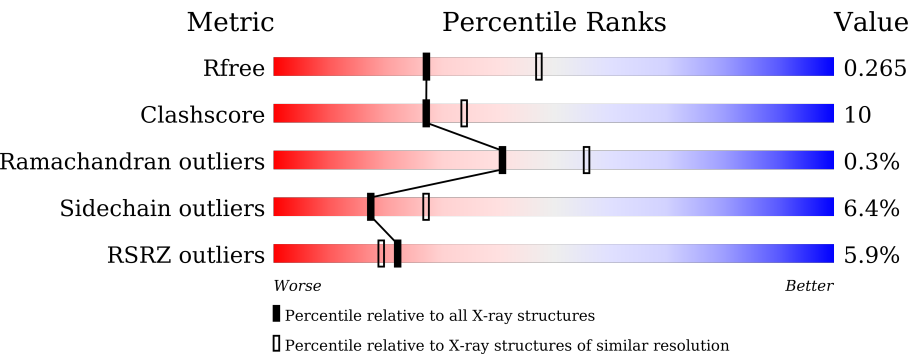
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	276	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>60%31%... .</div></div>
1	B	276	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>68%23%. 6%</div></div>
2	C	127	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>76%15%6%..</div></div>
2	D	127	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>80%15%. .</div></div>
2	E	127	<div><div>27%</div><div><div></div><div></div><div></div><div></div></div><div>63%28%. 5%</div></div>
2	F	127	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>70%24%. .</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8463 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 Putative GGDEF domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2130	1313	411	397	9			
1	B	260	Total	C	N	O	S	0	0	0
			2103	1294	407	393	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A069QEY1
B	0	SER	-	expression tag	UNP A0A069QEY1

- Molecule 2 is a protein called DUF1987 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	124	Total	C	N	O	S	0	0	0
			1007	631	177	195	4			
2	D	125	Total	C	N	O	S	0	0	0
			1015	636	178	196	5			
2	E	121	Total	C	N	O	S	0	0	0
			985	618	174	189	4			
2	F	122	Total	C	N	O	S	0	0	0
			993	624	175	190	4			

There are 4 discrepancies between the modelled and reference sequences:

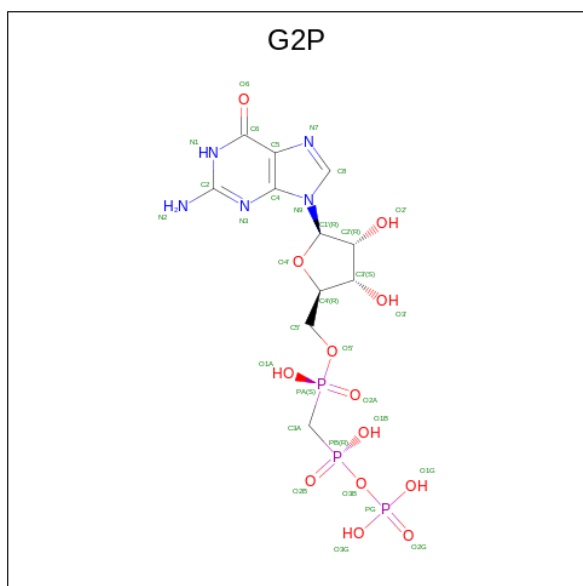
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP A0A072ZHB4
D	0	SER	-	expression tag	UNP A0A072ZHB4
E	0	SER	-	expression tag	UNP A0A072ZHB4
F	0	SER	-	expression tag	UNP A0A072ZHB4

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand

of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

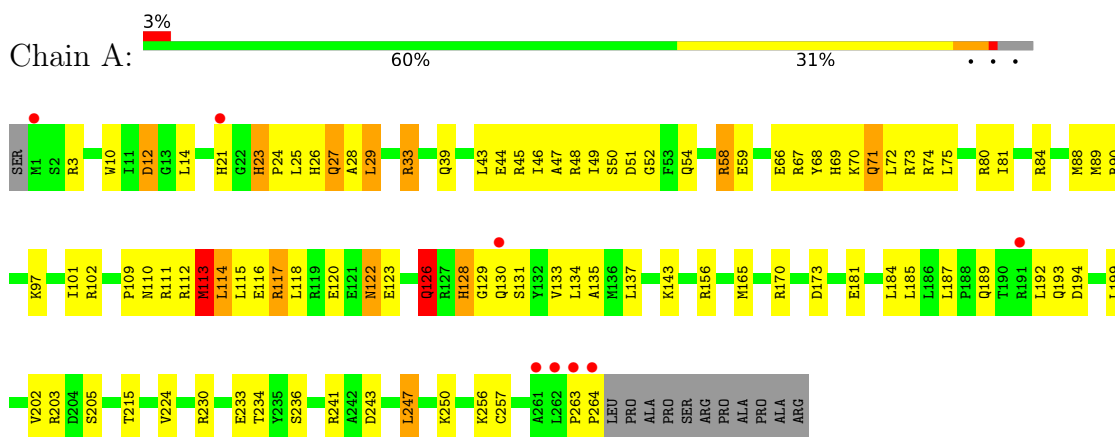
- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



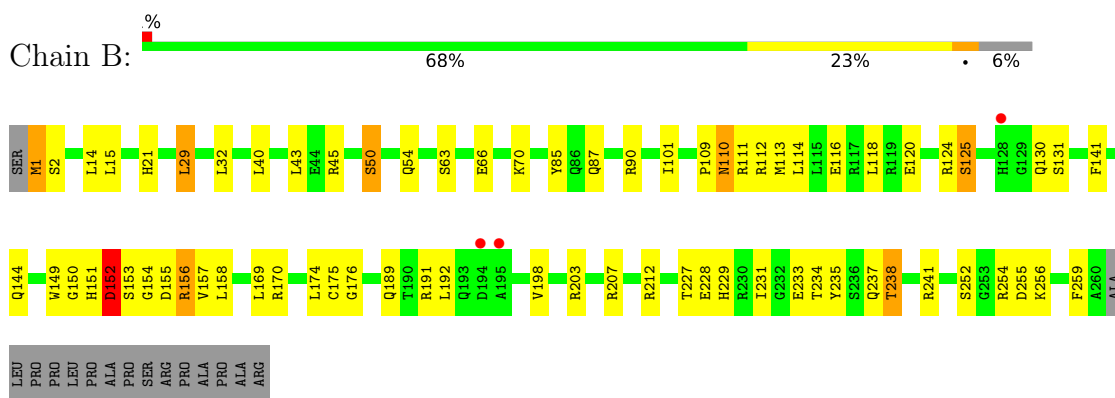
3 Residue-property plots [i](#)

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.

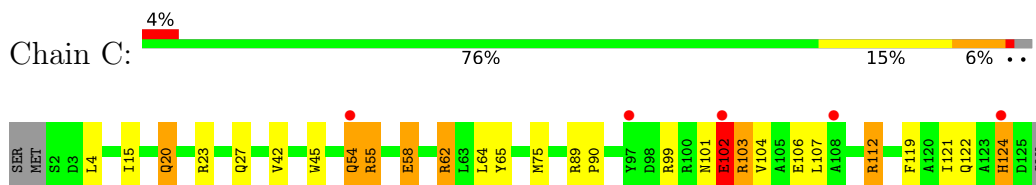
• Molecule 1: Putative GGDEF domain protein



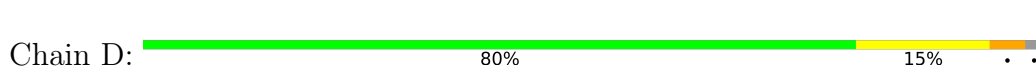
• Molecule 1: Putative GGDEF domain protein



• Molecule 2: DUF1987 domain-containing protein

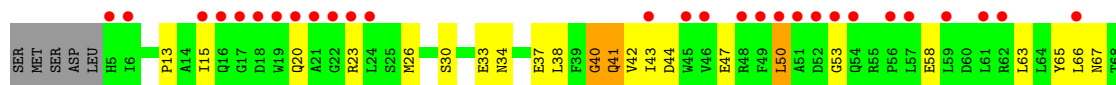


• Molecule 2: DUF1987 domain-containing protein

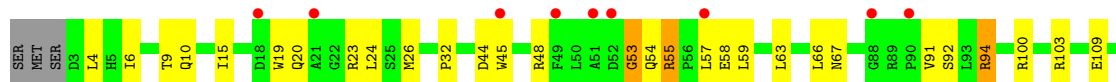




- Molecule 2: DUF1987 domain-containing protein



- Molecule 2: DUF1987 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	82.53Å 236.73Å 148.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.30 – 2.65 46.29 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.7 (46.30-2.65) 95.7 (46.29-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.218 , 0.265 0.220 , 0.265	Depositor DCC
R_{free} test set	2089 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8463	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: G2P, 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	A	1.67	63/2161 (2.9%)	0.98	11/2910 (0.4%)
1	B	1.27	32/2132 (1.5%)	0.88	5/2868 (0.2%)
2	C	1.25	11/1031 (1.1%)	0.93	3/1397 (0.2%)
2	D	1.11	12/1039 (1.2%)	0.72	0/1407
2	E	0.93	3/1009 (0.3%)	0.72	1/1367 (0.1%)
2	F	0.37	0/1017	0.63	0/1378
All	All	1.26	121/8389 (1.4%)	0.85	20/11327 (0.2%)

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
2	C	0	1
2	E	0	1
All	All	0	2

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ARG	CZ-NH2	-10.78	1.19	1.33
1	A	111	ARG	CZ-NH1	-10.34	1.19	1.33
2	D	110	GLU	CD-OE1	-10.08	1.14	1.25
2	D	5	HIS	C-O	-9.57	1.05	1.23
2	D	110	GLU	CD-OE2	-9.37	1.15	1.25
1	A	110	ASN	C-O	-9.01	1.06	1.23
1	A	84	ARG	C-O	-8.92	1.06	1.23
1	B	155	ASP	C-O	-8.85	1.06	1.23
1	A	67	ARG	C-O	-8.81	1.06	1.23
1	B	157	VAL	C-O	-8.78	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	75	MET	C-O	-8.71	1.06	1.23
1	A	112	ARG	C-O	-8.57	1.07	1.23
1	A	122	ASN	CG-OD1	-8.43	1.05	1.24
1	B	150	GLY	C-O	-8.38	1.10	1.23
1	A	27	GLN	C-O	-8.32	1.07	1.23
2	D	75	MET	CG-SD	-8.13	1.60	1.81
1	A	114	LEU	C-O	-8.03	1.08	1.23
1	A	80	ARG	C-O	-7.82	1.08	1.23
1	B	154	GLY	C-O	-7.78	1.11	1.23
1	A	73	ARG	C-O	-7.76	1.08	1.23
1	A	74	ARG	C-O	-7.72	1.08	1.23
2	D	110	GLU	C-O	-7.71	1.08	1.23
1	B	112	ARG	C-O	-7.69	1.08	1.23
1	B	156	ARG	C-O	-7.66	1.08	1.23
1	A	72	LEU	C-O	-7.64	1.08	1.23
1	A	47	ALA	C-O	-7.57	1.08	1.23
1	A	28	ALA	C-O	-7.45	1.09	1.23
1	A	116	GLU	C-O	-7.38	1.09	1.23
1	A	111	ARG	C-O	-7.23	1.09	1.23
1	B	153	SER	CB-OG	-7.22	1.32	1.42
1	A	110	ASN	CG-OD1	-7.04	1.08	1.24
1	B	203	ARG	CZ-NH1	-6.99	1.24	1.33
1	A	110	ASN	CG-ND2	-6.94	1.15	1.32
1	B	149	TRP	CB-CG	-6.87	1.37	1.50
1	B	158	LEU	C-O	-6.86	1.10	1.23
2	D	110	GLU	CG-CD	-6.85	1.41	1.51
1	A	59	GLU	C-O	-6.82	1.10	1.23
1	A	112	ARG	CZ-NH2	-6.80	1.24	1.33
1	B	151	HIS	C-O	-6.79	1.10	1.23
2	C	112	ARG	C-O	-6.78	1.10	1.23
1	A	70	LYS	C-O	-6.77	1.10	1.23
1	B	235	TYR	CE1-CZ	-6.66	1.29	1.38
1	B	238	THR	CB-CG2	-6.65	1.30	1.52
1	A	75	LEU	C-O	-6.57	1.10	1.23
1	B	152	ASP	C-O	-6.55	1.10	1.23
1	A	25	LEU	C-O	-6.51	1.10	1.23
2	D	10	GLN	C-O	-6.51	1.10	1.23
1	B	149	TRP	CE3-CZ3	-6.35	1.27	1.38
1	A	69	HIS	C-O	-6.32	1.11	1.23
1	A	109	PRO	C-O	-6.32	1.10	1.23
1	A	26	HIS	C-O	-6.30	1.11	1.23
1	A	29	LEU	C-O	-6.23	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ARG	C-O	-6.23	1.11	1.23
1	A	68	TYR	CB-CG	-6.19	1.42	1.51
1	B	110	ASN	CG-OD1	-6.16	1.10	1.24
2	E	82	GLU	CD-OE2	-6.14	1.18	1.25
1	A	50	SER	C-O	-6.13	1.11	1.23
1	A	48	ARG	C-O	-6.12	1.11	1.23
1	B	238	THR	C-O	-6.11	1.11	1.23
2	E	69	SER	CB-OG	-6.11	1.34	1.42
1	B	235	TYR	CG-CD1	-6.04	1.31	1.39
1	A	71	GLN	C-O	-6.02	1.11	1.23
1	A	143	LYS	C-O	-5.99	1.11	1.23
2	D	10	GLN	CA-CB	-5.96	1.40	1.53
2	C	65	TYR	C-O	-5.94	1.12	1.23
1	A	111	ARG	NE-CZ	-5.92	1.25	1.33
1	B	203	ARG	C-O	-5.92	1.12	1.23
1	B	235	TYR	C-O	-5.86	1.12	1.23
1	B	112	ARG	CZ-NH2	-5.84	1.25	1.33
1	A	52	GLY	C-O	-5.84	1.14	1.23
1	B	235	TYR	CZ-OH	-5.83	1.27	1.37
1	A	117	ARG	C-O	-5.82	1.12	1.23
1	A	84	ARG	CA-CB	-5.81	1.41	1.53
1	B	153	SER	C-O	-5.81	1.12	1.23
1	B	234	THR	N-CA	-5.81	1.34	1.46
1	A	49	ILE	C-O	-5.81	1.12	1.23
1	B	112	ARG	CZ-NH1	-5.80	1.25	1.33
1	A	46	ILE	C-O	-5.79	1.12	1.23
2	C	64	LEU	C-O	-5.75	1.12	1.23
1	A	143	LYS	N-CA	-5.75	1.34	1.46
1	A	80	ARG	N-CA	-5.72	1.34	1.46
1	A	68	TYR	C-O	-5.72	1.12	1.23
2	C	102	GLU	CD-OE2	-5.68	1.19	1.25
1	B	21	HIS	C-O	-5.67	1.12	1.23
2	C	58	GLU	CD-OE1	-5.66	1.19	1.25
1	A	115	LEU	C-O	-5.65	1.12	1.23
1	B	203	ARG	CZ-NH2	-5.62	1.25	1.33
1	A	74	ARG	CZ-NH2	-5.56	1.25	1.33
1	A	111	ARG	CA-CB	-5.53	1.41	1.53
1	B	149	TRP	CG-CD2	-5.49	1.34	1.43
1	A	126	GLN	C-O	-5.46	1.12	1.23
1	A	88	MET	CA-CB	-5.46	1.42	1.53
2	D	75	MET	CA-CB	-5.44	1.42	1.53
1	A	129	GLY	C-O	-5.43	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	ARG	N-CA	-5.42	1.35	1.46
1	A	66	GLU	C-O	-5.39	1.13	1.23
1	A	122	ASN	C-O	-5.39	1.13	1.23
1	A	114	LEU	N-CA	-5.39	1.35	1.46
1	B	144	GLN	C-O	-5.38	1.13	1.23
2	C	65	TYR	CZ-OH	-5.38	1.28	1.37
1	A	44	GLU	C-O	-5.35	1.13	1.23
2	C	101	ASN	C-O	-5.33	1.13	1.23
1	A	122	ASN	CG-ND2	-5.29	1.19	1.32
1	A	21	HIS	C-O	-5.28	1.13	1.23
1	A	113	MET	C-O	-5.26	1.13	1.23
1	A	114	LEU	CA-C	-5.26	1.39	1.52
1	A	58	ARG	C-O	-5.25	1.13	1.23
1	A	131	SER	C-O	-5.24	1.13	1.23
2	E	83	GLU	CD-OE2	-5.23	1.20	1.25
2	C	55	ARG	C-O	-5.22	1.13	1.23
2	C	58	GLU	C-O	-5.21	1.13	1.23
2	D	123	ALA	C-O	-5.20	1.13	1.23
1	A	71	GLN	CA-CB	-5.20	1.42	1.53
1	B	110	ASN	CG-ND2	-5.16	1.20	1.32
1	A	23	HIS	C-O	-5.14	1.13	1.23
1	B	111	ARG	C-O	-5.14	1.13	1.23
2	D	113	GLU	N-CA	-5.13	1.36	1.46
2	C	65	TYR	CE2-CZ	-5.11	1.31	1.38
1	A	51	ASP	C-O	-5.11	1.13	1.23
1	A	80	ARG	CD-NE	-5.11	1.37	1.46
2	C	104	VAL	C-O	-5.11	1.13	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ASP	CB-CG-OD2	15.08	131.87	118.30
1	A	112	ARG	NE-CZ-NH1	9.55	125.07	120.30
1	A	48	ARG	NE-CZ-NH1	-8.83	115.89	120.30
2	C	62	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	A	74	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	48	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	A	114	LEU	CA-CB-CG	-7.22	98.70	115.30
1	A	72	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	A	74	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	156	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	B	158	LEU	CA-CB-CG	5.83	128.72	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ASP	CB-CG-OD1	-5.83	113.05	118.30
2	E	40	GLY	C-N-CA	-5.79	107.22	121.70
1	B	158	LEU	CB-CG-CD2	5.67	120.64	111.00
1	A	75	LEU	CB-CG-CD2	5.62	120.55	111.00
1	A	72	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	25	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	143	LYS	N-CA-CB	-5.24	101.17	110.60
2	C	124	HIS	N-CA-CB	-5.23	101.19	110.60
2	C	104	VAL	CG1-CB-CG2	-5.20	102.59	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	99	ARG	Sidechain
2	E	102	GLU	Mainchain

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	2130	0	2137	33	0
1	B	2103	0	2107	47	0
2	C	1007	0	949	25	0
2	D	1015	0	961	14	0
2	E	985	0	929	30	0
2	F	993	0	940	23	0
3	A	1	0	0	0	0
4	A	32	0	12	3	0
5	A	72	0	0	2	0
5	B	40	0	0	2	0
5	C	25	0	0	0	0
5	D	49	0	0	3	0
5	E	3	0	0	1	0
5	F	8	0	0	0	0
All	All	8463	0	8035	164	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 (164) 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)
2:C:20:GLN:HA	2:C:55:ARG:HH22	1.20	1.07
2:C:62:ARG:NH1	2:C:124:HIS:CE1	2.29	1.01
1:B:191:ARG:HD3	1:B:228:GLU:OE1	1.60	1.00
2:E:50:LEU:HD21	2:E:84:ALA:HB2	1.41	0.99
2:C:62:ARG:HH12	2:C:124:HIS:CE1	1.87	0.90
2:E:33:GLU:OE2	2:E:33:GLU:N	2.05	0.89
1:A:234:THR:HG21	5:B:306:HOH:O	1.76	0.85
2:E:50:LEU:HD21	2:E:84:ALA:CB	2.05	0.85
2:C:62:ARG:HH12	2:C:124:HIS:HE1	1.29	0.81
2:C:20:GLN:HA	2:C:55:ARG:NH2	1.95	0.80
2:F:24:LEU:HB3	2:F:59:LEU:HD22	1.65	0.78
2:E:50:LEU:CD2	2:E:84:ALA:HB2	2.14	0.77
1:A:130:GLN:OE1	1:A:189:GLN:HG2	1.86	0.75
1:B:192:LEU:HD23	1:B:259:PHE:HD2	1.51	0.75
2:D:125:ASP:OD1	2:D:125:ASP:N	2.15	0.75
1:A:81:ILE:HG12	2:D:110:GLU:HG2	1.70	0.73
2:E:94:ARG:HG2	2:E:120:ALA:HB3	1.71	0.72
1:B:152:ASP:OD1	1:B:152:ASP:N	2.17	0.71
2:F:15:ILE:HG12	2:F:26:MET:HG2	1.72	0.71
2:E:34:ASN:HB3	2:E:37:GLU:HG2	1.73	0.70
2:C:20:GLN:CA	2:C:55:ARG:HH22	2.02	0.69
1:A:250:LYS:HE3	4:A:302:G2P:O1G	1.92	0.69
1:B:233:GLU:OE1	1:B:237:GLN:HG3	1.93	0.68
2:F:20:GLN:O	2:F:55:ARG:NH2	2.27	0.66
1:B:169:LEU:HD11	1:B:175:CYS:HB2	1.77	0.66
2:E:23:ARG:NH1	2:E:58:GLU:OE1	2.29	0.65
2:C:62:ARG:HH11	2:C:124:HIS:CE1	2.13	0.65
1:B:191:ARG:NH1	1:B:228:GLU:OE1	2.24	0.64
1:A:12:ASP:OD2	1:A:33:ARG:NH2	2.31	0.63
2:D:23:ARG:NH1	5:D:202:HOH:O	2.31	0.63
1:A:233:GLU:OE1	1:A:241:ARG:NH2	2.27	0.62
2:F:92:SER:HB2	2:F:118:PRO:HB2	1.83	0.61
1:B:141:PHE:HE2	1:B:254:ARG:HD2	1.66	0.59
2:F:109:GLU:OE2	2:F:112:ARG:NE	2.36	0.58
2:C:23:ARG:HH11	2:C:23:ARG:HG3	1.69	0.58
2:E:106:GLU:O	2:E:107:LEU:C	2.39	0.57
2:D:15:ILE:HG12	2:D:26:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:ARG:HH11	2:F:122:GLN:NE2	2.02	0.57
2:F:53:GLY:O	2:F:55:ARG:N	2.38	0.57
1:B:170:ARG:HE	1:B:198:VAL:HG21	1.70	0.56
1:A:243:ASP:OD2	1:B:212:ARG:HD3	2.05	0.56
1:A:134:LEU:HG	1:A:184:LEU:HD11	1.88	0.56
1:A:250:LYS:CE	4:A:302:G2P:O1G	2.53	0.56
1:B:192:LEU:HD23	1:B:259:PHE:CD2	2.36	0.56
2:C:112:ARG:HH21	2:C:121:ILE:HD12	1.70	0.56
1:B:156:ARG:NH1	1:B:212:ARG:O	2.35	0.56
1:B:1:MET:HE3	1:B:2:SER:H	1.69	0.55
1:B:110:ASN:OD1	1:B:113:MET:HG3	2.05	0.55
1:B:238:THR:HG22	1:B:238:THR:O	2.04	0.55
2:F:9:THR:HG22	2:F:10:GLN:H	1.71	0.55
2:E:96:HIS:HA	2:E:122:GLN:O	2.05	0.55
1:B:101:ILE:HB	1:B:113:MET:SD	2.47	0.54
2:F:58:GLU:HA	2:F:92:SER:O	2.08	0.54
1:A:199:LEU:O	1:A:203:ARG:HG3	2.08	0.54
1:B:233:GLU:HB3	5:B:312:HOH:O	2.08	0.54
2:E:99:ARG:HG2	2:E:123:ALA:HB1	1.90	0.54
2:C:112:ARG:NH2	2:C:121:ILE:HD12	2.23	0.53
2:E:65:TYR:O	2:E:66:LEU:HD23	2.07	0.53
1:A:101:ILE:HB	1:A:113:MET:HG3	1.91	0.53
2:F:94:ARG:HH11	2:F:122:GLN:HE21	1.55	0.53
1:B:85:TYR:CZ	2:C:107:LEU:HD23	2.44	0.53
1:B:233:GLU:HG2	1:B:237:GLN:HB2	1.91	0.53
2:C:102:GLU:H	2:C:102:GLU:CD	2.08	0.53
1:A:23:HIS:ND1	1:A:24:PRO:HD2	2.24	0.53
1:A:123:GLU:O	1:A:126:GLN:HB2	2.09	0.52
1:A:230:ARG:O	1:A:233:GLU:HB3	2.08	0.52
1:A:241:ARG:NE	5:A:402:HOH:O	2.24	0.52
2:E:26:MET:HB3	2:E:63:LEU:HD21	1.93	0.51
2:F:23:ARG:HH11	2:F:58:GLU:CD	2.14	0.51
1:B:125:SER:O	1:B:231:ILE:CD1	2.59	0.51
2:C:102:GLU:HG2	2:C:103:ARG:HG2	1.91	0.51
2:E:41:GLN:O	2:E:42:VAL:C	2.47	0.50
1:A:128:HIS:N	1:A:128:HIS:ND1	2.59	0.49
2:E:89:ARG:HD2	2:E:90:PRO:HD2	1.94	0.49
2:E:43:ILE:O	2:E:47:GLU:HG2	2.12	0.49
2:E:58:GLU:OE2	2:E:94:ARG:NH2	2.45	0.49
1:A:247:LEU:HG	1:B:212:ARG:HG2	1.95	0.49
1:A:165:MET:HG2	1:A:202:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG22	1:A:187:LEU:HB2	1.95	0.49
1:B:125:SER:O	1:B:231:ILE:HD13	2.13	0.48
1:B:114:LEU:HD21	1:B:176:GLY:HA3	1.95	0.48
1:A:54:GLN:OE1	2:E:67:ASN:HA	2.14	0.48
2:C:23:ARG:HG3	2:C:23:ARG:NH1	2.29	0.48
2:F:100:ARG:HH21	2:F:100:ARG:HG3	1.79	0.48
1:A:10:TRP:O	1:A:14:LEU:HD13	2.14	0.47
1:B:192:LEU:HD11	1:B:228:GLU:HB2	1.96	0.47
2:F:6:ILE:HG23	2:F:15:ILE:HB	1.96	0.47
1:A:117:ARG:HA	1:A:120:GLU:HG2	1.95	0.47
2:C:103:ARG:HA	2:C:106:GLU:OE1	2.14	0.47
1:A:39:GLN:O	1:A:43:LEU:HD13	2.15	0.46
1:B:50:SER:O	1:B:54:GLN:HG2	2.15	0.46
2:F:6:ILE:CG2	2:F:15:ILE:HB	2.44	0.46
2:E:37:GLU:O	2:E:41:GLN:NE2	2.48	0.46
2:F:32:PRO:HD2	2:F:67:ASN:ND2	2.29	0.46
2:F:63:LEU:HB3	2:F:66:LEU:HD11	1.98	0.46
1:A:156:ARG:HD2	5:A:461:HOH:O	2.16	0.46
2:D:74:MET:O	2:D:78:LEU:HG	2.16	0.46
2:F:57:LEU:O	2:F:91:VAL:HA	2.15	0.46
2:E:15:ILE:HG12	2:E:26:MET:HG2	1.98	0.46
2:D:58:GLU:HG2	5:D:202:HOH:O	2.15	0.45
1:B:66:GLU:O	1:B:70:LYS:HG3	2.16	0.45
1:B:227:THR:OG1	1:B:228:GLU:N	2.46	0.45
2:F:103:ARG:HE	2:F:103:ARG:HB3	1.48	0.45
1:B:90:ARG:NH2	2:D:10:GLN:O	2.50	0.45
1:A:224:VAL:O	1:A:257:CYS:HA	2.17	0.45
1:B:131:SER:HB2	1:B:229:HIS:HB3	1.99	0.45
2:E:40:GLY:O	2:E:41:GLN:C	2.50	0.45
1:B:87:GLN:HG3	2:C:103:ARG:HH22	1.81	0.45
2:D:29:ASP:OD1	2:D:64:LEU:HB2	2.17	0.44
2:C:103:ARG:HG2	2:C:103:ARG:H	1.42	0.44
1:A:234:THR:HG23	1:A:236:SER:H	1.83	0.44
1:B:191:ARG:HH11	1:B:228:GLU:CD	2.17	0.43
2:C:27:GLN:HA	2:C:62:ARG:O	2.17	0.43
1:B:101:ILE:O	1:B:113:MET:SD	2.76	0.43
2:C:4:LEU:HB2	2:C:45:TRP:CD1	2.52	0.43
1:B:40:LEU:HD12	1:B:40:LEU:HA	1.79	0.43
1:B:228:GLU:O	1:B:241:ARG:NH2	2.43	0.43
1:A:135:ALA:HB3	1:A:185:LEU:HB2	1.99	0.43
1:A:250:LYS:NZ	4:A:302:G2P:O1G	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:HD12	1:A:192:LEU:HA	1.87	0.43
2:D:26:MET:HE1	2:D:39:PHE:HE1	1.83	0.43
1:B:116:GLU:O	1:B:120:GLU:HG3	2.19	0.43
1:B:207:ARG:NH1	1:B:255:ASP:OD1	2.52	0.43
2:F:94:ARG:HD3	2:F:122:GLN:HE21	1.84	0.43
1:A:29:LEU:O	1:A:29:LEU:HG	2.18	0.42
1:B:124:ARG:HH11	1:B:189:GLN:NE2	2.17	0.42
2:D:91:VAL:O	2:D:118:PRO:HD2	2.19	0.42
1:B:87:GLN:HG3	2:C:103:ARG:NH2	2.34	0.42
1:B:227:THR:HG23	1:B:228:GLU:N	2.33	0.42
2:E:34:ASN:CB	2:E:37:GLU:HG2	2.46	0.42
2:D:19:TRP:CH2	2:D:49:PHE:HA	2.54	0.42
2:E:96:HIS:ND1	2:E:122:GLN:HB3	2.34	0.42
2:E:112:ARG:O	2:E:112:ARG:HG2	2.16	0.42
1:A:170:ARG:HD3	1:A:173:ASP:OD2	2.19	0.42
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.92	0.42
2:E:41:GLN:O	2:E:44:ASP:N	2.53	0.42
2:C:89:ARG:HD2	2:C:90:PRO:HD2	2.01	0.42
2:C:112:ARG:O	2:C:112:ARG:CG	2.67	0.42
2:E:20:GLN:H	2:E:20:GLN:HG2	1.58	0.42
2:D:20:GLN:NE2	5:D:204:HOH:O	2.52	0.42
1:A:263:PRO:HA	1:A:264:PRO:HD3	1.94	0.42
1:B:109:PRO:HD2	1:B:175:CYS:O	2.19	0.42
2:C:23:ARG:HH12	2:C:58:GLU:CD	2.23	0.41
2:E:15:ILE:HD13	2:E:42:VAL:HG21	2.01	0.41
2:F:4:LEU:HB2	2:F:45:TRP:CD1	2.55	0.41
2:C:15:ILE:HD13	2:C:42:VAL:HG21	2.02	0.41
2:D:58:GLU:OE1	2:D:94:ARG:NH1	2.51	0.41
1:B:191:ARG:HD3	1:B:228:GLU:CD	2.36	0.41
2:D:23:ARG:NH1	2:D:58:GLU:OE1	2.53	0.41
2:E:13:PRO:HD3	2:E:30:SER:HA	2.03	0.41
2:E:105:ALA:O	2:E:106:GLU:C	2.52	0.41
1:B:252:SER:O	1:B:252:SER:OG	2.37	0.41
1:A:118:LEU:HD21	1:A:134:LEU:HD11	2.02	0.41
1:B:191:ARG:NH1	1:B:228:GLU:CD	2.73	0.41
2:F:44:ASP:O	2:F:48:ARG:HG3	2.21	0.41
1:B:15:LEU:HD21	1:B:29:LEU:HB3	2.03	0.41
1:B:43:LEU:O	1:B:43:LEU:HD23	2.21	0.41
2:F:100:ARG:HG3	2:F:100:ARG:NH2	2.36	0.41
1:B:54:GLN:HG2	1:B:54:GLN:H	1.73	0.41
2:E:34:ASN:HB3	2:E:37:GLU:CG	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:109:GLU:O	2:F:112:ARG:N	2.54	0.40
1:B:1:MET:HE2	1:B:1:MET:HB3	1.80	0.40
2:E:100:ARG:NH1	5:E:201:HOH:O	2.53	0.40
2:C:54:GLN:HA	2:C:89:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/276 (95%)	257 (98%)	5 (2%)	0	100	100
1	B	258/276 (94%)	252 (98%)	6 (2%)	0	100	100
2	C	122/127 (96%)	115 (94%)	7 (6%)	0	100	100
2	D	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
2	E	119/127 (94%)	112 (94%)	6 (5%)	1 (1%)	19	29
2	F	120/127 (94%)	114 (95%)	4 (3%)	2 (2%)	9	13
All	All	1004/1060 (95%)	970 (97%)	31 (3%)	3 (0%)	41	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	54	GLN
2	E	53	GLY
2	F	53	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	A	227/236 (96%)	204 (90%)	23 (10%)	7	10
1	B	224/236 (95%)	212 (95%)	12 (5%)	22	34
2	C	107/110 (97%)	100 (94%)	7 (6%)	17	26
2	D	108/110 (98%)	103 (95%)	5 (5%)	27	41
2	E	104/110 (94%)	99 (95%)	5 (5%)	25	39
2	F	105/110 (96%)	101 (96%)	4 (4%)	33	49
All	All	875/912 (96%)	819 (94%)	56 (6%)	17	27

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	12	ASP
1	A	27	GLN
1	A	33	ARG
1	A	58	ARG
1	A	71	GLN
1	A	89	MET
1	A	90	ARG
1	A	97	LYS
1	A	102	ARG
1	A	113	MET
1	A	114	LEU
1	A	122	ASN
1	A	126	GLN
1	A	128	HIS
1	A	137	LEU
1	A	181	GLU
1	A	193	GLN
1	A	194	ASP
1	A	205	SER
1	A	215	THR
1	A	247	LEU
1	A	256	LYS
1	B	1	MET
1	B	14	LEU
1	B	29	LEU

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Mol	Chain	Res	Type
1	B	32	LEU
1	B	45	ARG
1	B	50	SER
1	B	63	SER
1	B	125	SER
1	B	130	GLN
1	B	152	ASP
1	B	174	LEU
1	B	256	LYS
2	C	20	GLN
2	C	54	GLN
2	C	75	MET
2	C	102	GLU
2	C	103	ARG
2	C	119	PHE
2	C	122	GLN
2	D	35	SER
2	D	58	GLU
2	D	75	MET
2	D	119	PHE
2	D	125	ASP
2	E	38	LEU
2	E	41	GLN
2	E	50	LEU
2	E	82	GLU
2	E	112	ARG
2	F	19	TRP
2	F	55	ARG
2	F	94	ARG
2	F	116	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	34	GLN
1	B	93	ASN
1	B	144	GLN
1	B	229	HIS
2	C	124	HIS
2	F	122	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
4	G2P	A	302	3	26,34,34	5.80	22 (84%)	30,54,54	2.76	13 (43%)

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
4	G2P	A	302	3	-	5/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	G2P	C4-N9	-13.83	1.29	1.47
4	A	302	G2P	C5-C6	-12.51	1.31	1.52
4	A	302	G2P	PB-O1B	-11.13	1.30	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	G2P	PB-O2B	-7.53	1.33	1.51
4	A	302	G2P	PA-O1A	-7.21	1.39	1.56
4	A	302	G2P	PG-O2G	-6.21	1.30	1.50
4	A	302	G2P	PG-O1G	-6.11	1.31	1.54
4	A	302	G2P	O4'-C4'	-5.94	1.31	1.45
4	A	302	G2P	PA-O5'	-5.72	1.48	1.57
4	A	302	G2P	PG-O3G	-5.48	1.33	1.54
4	A	302	G2P	C8-N9	-4.62	1.29	1.45
4	A	302	G2P	O4'-C1'	-4.07	1.32	1.42
4	A	302	G2P	C3'-C4'	-3.59	1.43	1.53
4	A	302	G2P	C2'-C1'	-3.50	1.42	1.53
4	A	302	G2P	C5-C4	-3.21	1.33	1.53
4	A	302	G2P	PA-O2A	-2.99	1.44	1.51
4	A	302	G2P	C2-N2	-2.69	1.23	1.36
4	A	302	G2P	O2'-C2'	-2.52	1.37	1.43
4	A	302	G2P	C6-N1	2.49	1.37	1.33
4	A	302	G2P	C2-N1	-2.29	1.34	1.44
4	A	302	G2P	O3'-C3'	-2.20	1.37	1.43
4	A	302	G2P	O6-C6	-2.03	1.19	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	G2P	O4'-C1'-C2'	-6.91	91.57	106.64
4	A	302	G2P	O2A-PA-C3A	-6.67	91.45	109.07
4	A	302	G2P	O1A-PA-C3A	-5.90	82.42	106.58
4	A	302	G2P	O6-C6-N1	-4.28	116.93	122.69
4	A	302	G2P	O1A-PA-O2A	3.84	122.89	110.07
4	A	302	G2P	O4'-C4'-C3'	-3.36	98.47	105.11
4	A	302	G2P	C4-C5-N7	2.98	106.41	102.46
4	A	302	G2P	PG-O3B-PB	2.69	142.07	132.62
4	A	302	G2P	O2B-PB-C3A	-2.43	102.65	109.07
4	A	302	G2P	O4'-C4'-C5'	-2.41	101.45	109.37
4	A	302	G2P	C4'-O4'-C1'	-2.20	104.62	109.47
4	A	302	G2P	O6-C6-C5	2.16	124.27	119.86
4	A	302	G2P	O3G-PG-O1G	2.00	115.29	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	G2P	PB-C3A-PA-O1A

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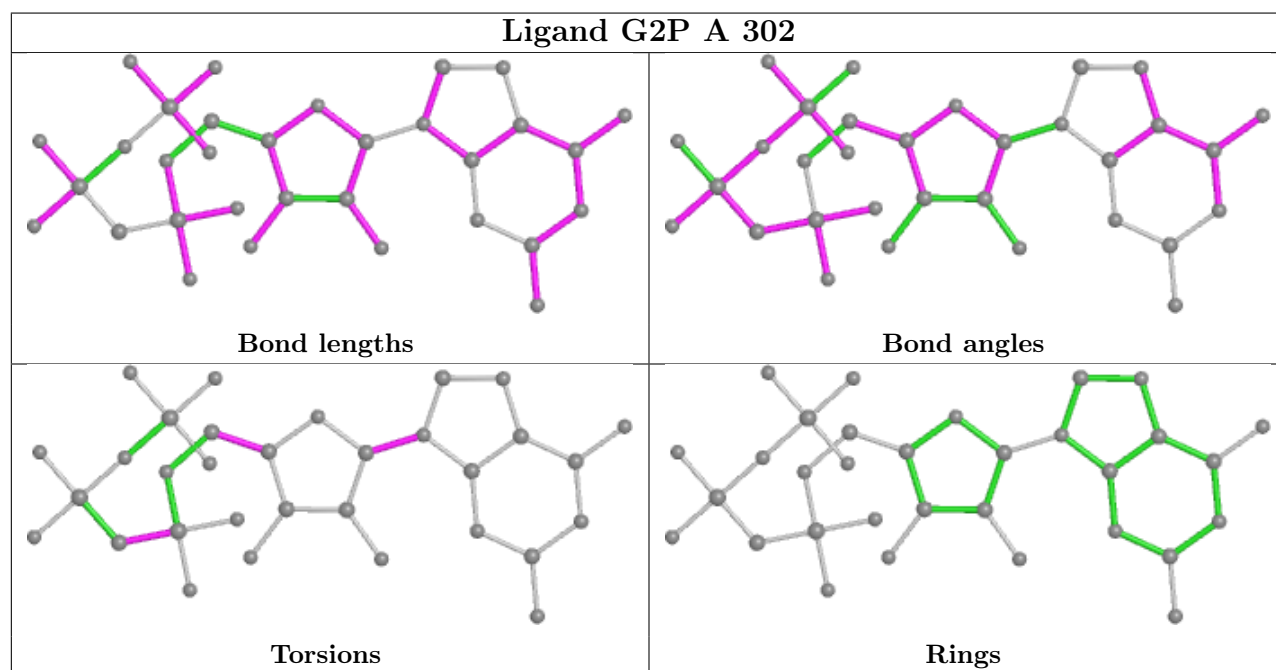
Mol	Chain	Res	Type	Atoms
4	A	302	G2P	PB-C3A-PA-O2A
4	A	302	G2P	PB-C3A-PA-O5'
4	A	302	G2P	O4'-C4'-C5'-O5'
4	A	302	G2P	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	G2P	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 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	264/276 (95%)	0.12	8 (3%)	50	47	19, 42, 70, 115	0
1	B	260/276 (94%)	0.03	3 (1%)	79	77	23, 50, 78, 102	0
2	C	124/127 (97%)	0.26	5 (4%)	38	34	26, 51, 80, 102	0
2	D	125/127 (98%)	-0.11	0	100	100	16, 27, 54, 69	0
2	E	121/127 (95%)	1.37	34 (28%)	0	0	51, 96, 127, 131	0
2	F	122/127 (96%)	0.60	10 (8%)	11	9	41, 74, 102, 108	0
All	All	1016/1060 (95%)	0.29	60 (5%)	22	19	16, 50, 102, 131	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	51	ALA	6.2
2	E	53	GLY	5.4
2	E	50	LEU	4.6
2	E	49	PHE	4.4
2	E	57	LEU	4.3
2	F	21	ALA	4.3
2	E	56	PRO	4.2
2	E	59	LEU	3.8
2	E	45	TRP	3.7
1	A	1	MET	3.7
2	E	52	ASP	3.7
2	E	94	ARG	3.6
2	E	15	ILE	3.6
1	A	264	PRO	3.6
1	A	261	ALA	3.5
2	E	43	ILE	3.4
2	E	18	ASP	3.4
2	E	6	ILE	3.3
2	E	24	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	90	PRO	3.1
2	F	51	ALA	3.0
2	E	17	GLY	3.0
2	E	48	ARG	3.0
2	E	46	VAL	3.0
2	F	49	PHE	3.0
2	E	95	TRP	2.9
2	E	21	ALA	2.9
2	E	20	GLN	2.9
1	A	262	LEU	2.9
1	A	263	PRO	2.9
1	B	195	ALA	2.8
2	E	23	ARG	2.8
2	E	91	VAL	2.7
1	A	191	ARG	2.7
1	A	130	GLN	2.6
2	C	97	TYR	2.6
2	E	87	GLY	2.5
2	E	5	HIS	2.5
2	E	22	GLY	2.4
1	B	194	ASP	2.4
2	F	88	GLY	2.4
2	F	52	ASP	2.3
1	B	128	HIS	2.3
2	E	62	ARG	2.3
2	F	45	TRP	2.2
2	C	102	GLU	2.2
2	F	116	SER	2.2
2	C	124	HIS	2.1
2	E	16	GLN	2.1
2	E	54	GLN	2.1
2	F	57	LEU	2.1
2	E	61	LEU	2.1
1	A	21	HIS	2.1
2	E	66	LEU	2.1
2	C	108	ALA	2.1
2	E	119	PHE	2.1
2	C	54	GLN	2.1
2	F	18	ASP	2.0
2	E	19	TRP	2.0
2	E	81	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

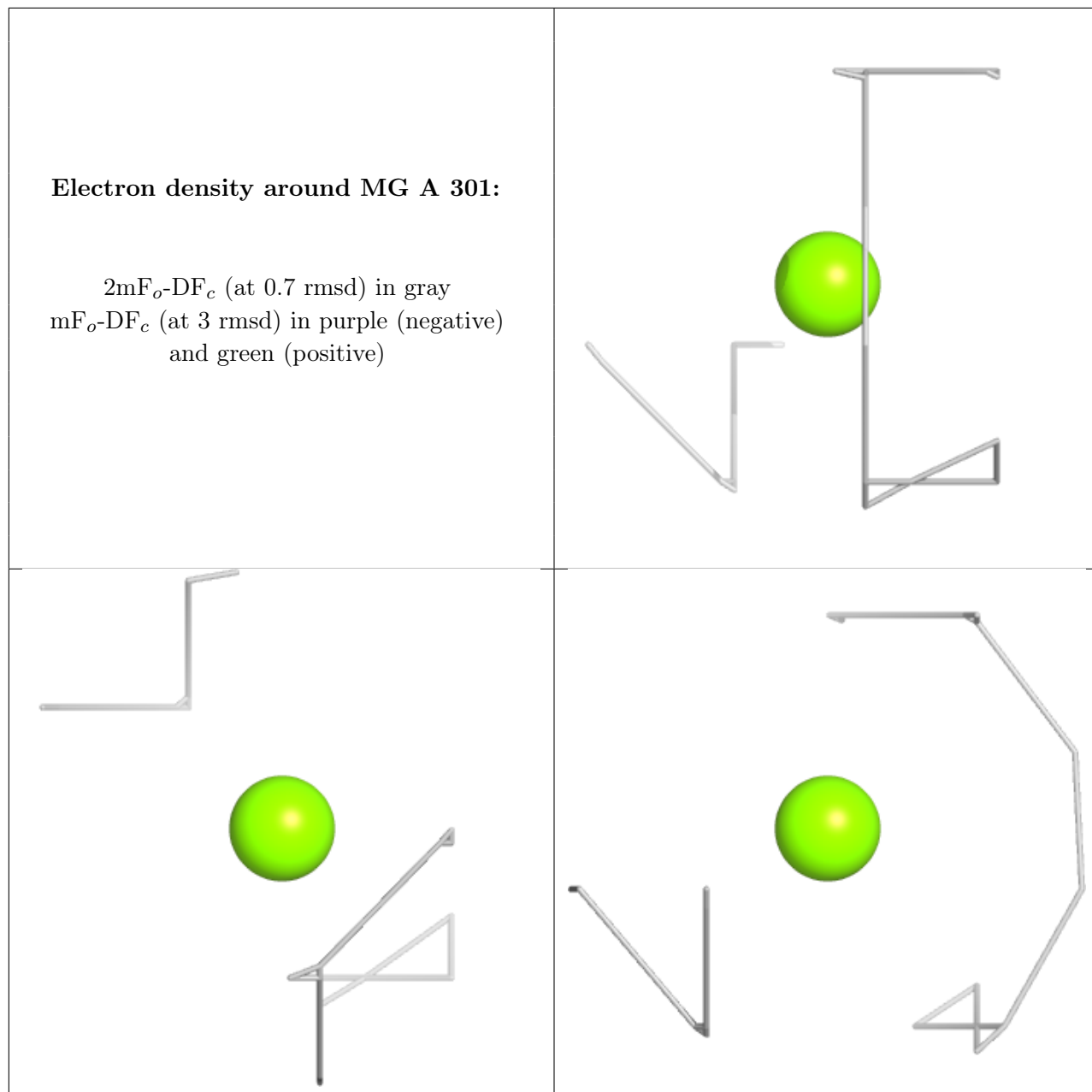
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	301	1/1	0.95	0.18	28,28,28,28	0
4	G2P	A	302	32/32	0.96	0.14	35,51,68,99	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.

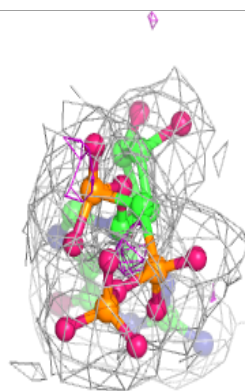
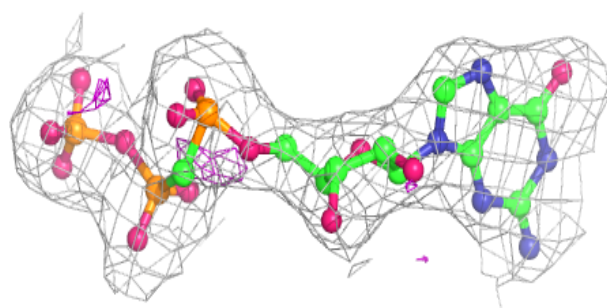
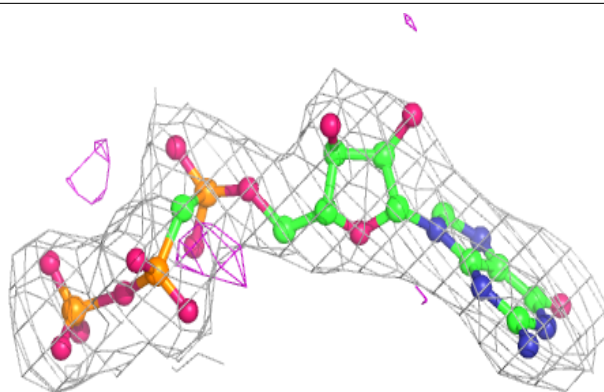
Electron density around MG A 301:

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



Electron density around G2P A 302:

$2mF_o-DF_c$ (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.