



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:52 PM UTC

PDB ID : 7E6G / pdb_00007e6g
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 types of validation reports are described at

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

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

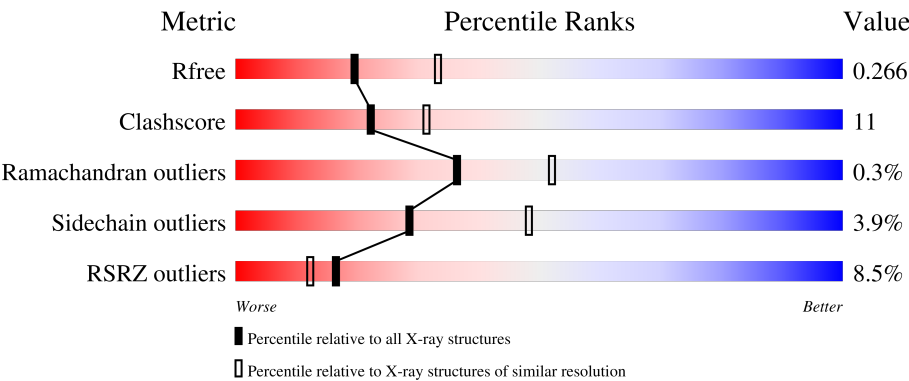
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	4% 58% 32% 5%
1	B	276	3% 66% 23% 6%
2	C	127	4% 69% 20% 6%
2	D	127	% 80% 14% 5%
2	E	127	34% 61% 27% 6% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	127	16% 72% 24%

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:

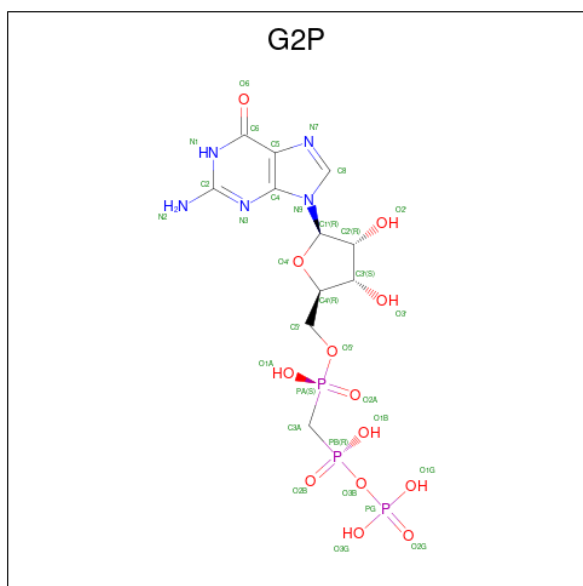
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP A0A072ZHB4
D	0	SER	-	expression tag	UNP A0A072ZHB4
E	0	SER	-	expression tag	UNP A0A072ZHB4
F	0	SER	-	expression tag	UNP A0A072ZHB4

- Molecule 3 is MAGNESIUM ION (CCD ID: 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 (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0
			32	11	5	13	3	0

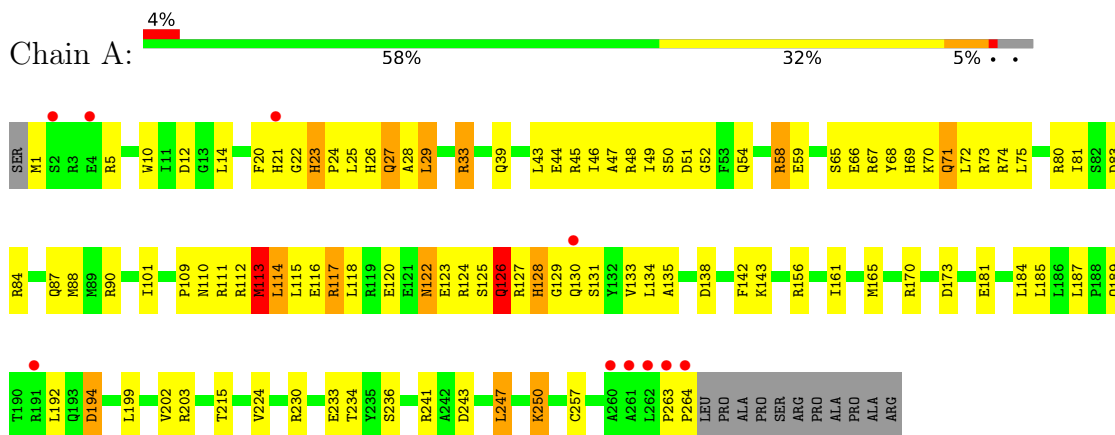
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	40	Total	O	0	0
			40	40		
5	C	25	Total	O	0	0
			25	25		
5	D	49	Total	O	0	0
			49	49		
5	E	3	Total	O	0	0
			3	3		
5	F	8	Total	O	0	0
			8	8		

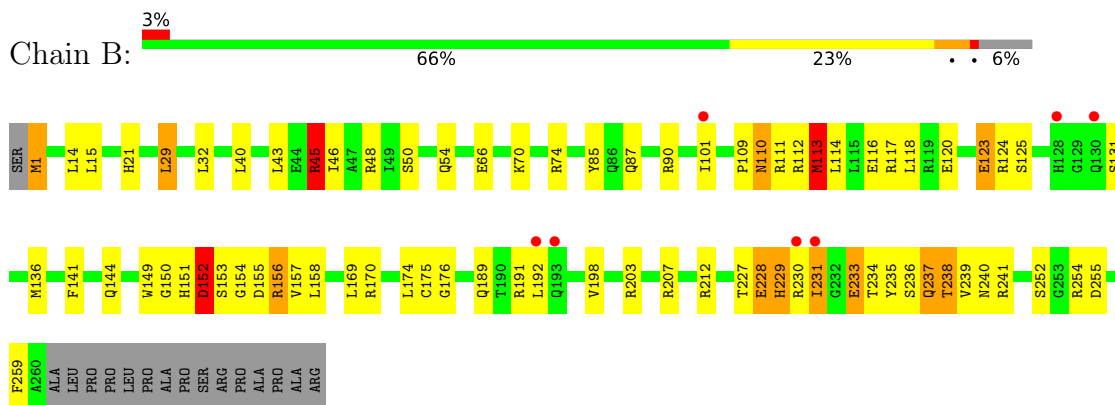
3 Residue-property plots [i](#)

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.

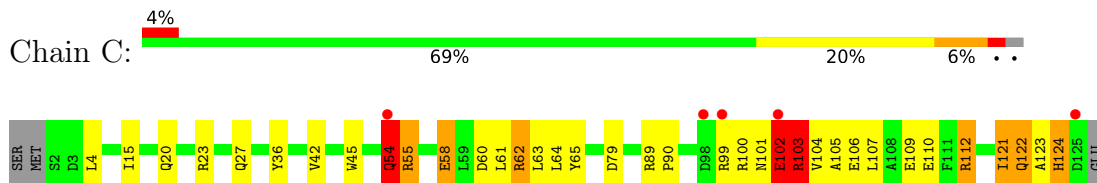
- Molecule 1: Putative GGDEF domain protein



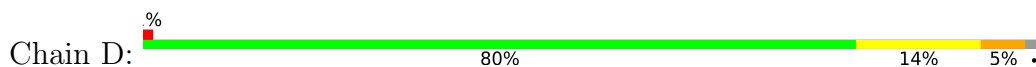
- Molecule 1: Putative GGDEF domain protein



- Molecule 2: DUF1987 domain-containing protein

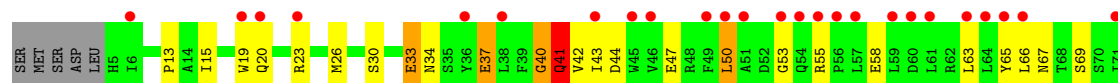


- Molecule 2: DUF1987 domain-containing protein

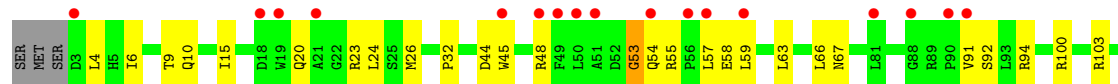




- Molecule 2: DUF1987 domain-containing protein



- 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 46.30 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.7 (46.30-2.65) 95.7 (46.30-2.65)	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 0.219 , 0.266	Depositor DCC
R_{free} test set	2089 reflections (4.89%)	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)	0.35 , 54.0	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: MG, G2P

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	2.47	147/2161 (6.8%)	1.09	12/2910 (0.4%)
1	B	1.75	75/2132 (3.5%)	0.95	8/2868 (0.3%)
2	C	1.70	34/1031 (3.3%)	1.07	9/1397 (0.6%)
2	D	1.44	25/1039 (2.4%)	0.75	2/1407 (0.1%)
2	E	1.27	23/1009 (2.3%)	0.93	6/1367 (0.4%)
2	F	0.30	0/1017	0.60	0/1378
All	All	1.78	304/8389 (3.6%)	0.95	37/11327 (0.3%)

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 (304) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	HIS	C-O	-16.66	1.05	1.24
1	A	110	ASN	C-O	-15.18	1.06	1.23
1	A	84	ARG	C-O	-15.14	1.06	1.24
1	B	155	ASP	C-O	-15.03	1.06	1.24
1	A	67	ARG	C-O	-14.71	1.06	1.24
1	B	157	VAL	C-O	-14.67	1.06	1.24
1	A	112	ARG	C-O	-14.58	1.07	1.24
2	D	75	MET	C-O	-14.55	1.06	1.24
1	A	114	LEU	C-O	-13.46	1.08	1.24
1	A	80	ARG	C-O	-13.46	1.08	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	ARG	C-O	-13.36	1.08	1.24
1	A	74	ARG	C-O	-13.20	1.08	1.24
1	A	27	GLN	C-O	-13.12	1.07	1.24
1	A	72	LEU	C-O	-13.07	1.08	1.24
1	A	73	ARG	C-O	-13.02	1.08	1.24
2	D	110	GLU	C-O	-12.94	1.08	1.24
1	A	28	ALA	C-O	-12.76	1.09	1.24
1	A	47	ALA	C-O	-12.72	1.08	1.24
1	A	116	GLU	C-O	-12.43	1.09	1.24
1	A	111	ARG	C-O	-12.40	1.09	1.24
1	B	156	ARG	C-O	-12.14	1.08	1.24
1	A	59	GLU	C-O	-11.92	1.10	1.24
1	B	158	LEU	C-O	-11.80	1.10	1.24
1	A	70	LYS	C-O	-11.65	1.10	1.24
1	A	109	PRO	C-O	-11.57	1.10	1.23
1	A	75	LEU	C-O	-11.51	1.10	1.24
1	B	152	ASP	C-O	-11.30	1.10	1.24
1	A	111	ARG	CZ-NH2	-11.09	1.19	1.33
1	A	26	HIS	C-O	-10.98	1.11	1.24
1	B	151	HIS	C-O	-10.91	1.10	1.24
1	B	150	GLY	C-O	-10.77	1.10	1.23
1	A	69	HIS	C-O	-10.73	1.11	1.24
1	A	50	SER	C-O	-10.61	1.11	1.24
1	A	29	LEU	C-O	-10.59	1.11	1.24
1	A	45	ARG	C-O	-10.59	1.11	1.24
1	B	238	THR	C-O	-10.59	1.11	1.24
1	B	154	GLY	C-O	-10.50	1.11	1.23
1	A	114	LEU	CA-C	-10.48	1.39	1.52
1	A	71	GLN	C-O	-10.44	1.11	1.24
1	A	48	ARG	C-O	-10.41	1.11	1.24
1	A	143	LYS	C-O	-10.38	1.11	1.24
2	C	112	ARG	C-O	-10.17	1.10	1.24
1	A	46	ILE	C-O	-10.10	1.12	1.24
1	B	203	ARG	C-O	-10.10	1.12	1.24
1	A	68	TYR	C-O	-9.95	1.12	1.24
1	A	49	ILE	C-O	-9.94	1.12	1.24
1	B	153	SER	C-O	-9.92	1.12	1.24
2	D	10	GLN	C-O	-9.88	1.10	1.24
1	A	126	GLN	C-O	-9.68	1.12	1.24
1	A	115	LEU	C-O	-9.67	1.12	1.24
2	C	65	TYR	C-O	-9.61	1.12	1.23
1	A	80	ARG	N-CA	-9.56	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ASN	CG-OD1	-9.54	1.05	1.23
1	A	116	GLU	CA-C	-9.51	1.40	1.52
1	B	235	TYR	C-O	-9.51	1.12	1.24
1	A	143	LYS	N-CA	-9.50	1.34	1.46
1	B	21	HIS	C-O	-9.49	1.12	1.23
1	A	73	ARG	CA-C	-9.47	1.40	1.52
1	A	25	LEU	C-O	-9.38	1.10	1.23
1	A	111	ARG	CZ-NH1	-9.39	1.19	1.32
1	A	122	ASN	C-O	-9.25	1.13	1.24
2	C	58	GLU	C-O	-9.23	1.13	1.24
1	B	144	GLN	C-O	-9.22	1.13	1.24
1	A	113	MET	C-O	-9.20	1.13	1.24
2	C	64	LEU	C-O	-9.17	1.12	1.24
1	B	112	ARG	N-CA	-9.14	1.35	1.46
1	A	117	ARG	C-O	-9.12	1.12	1.24
1	A	47	ALA	CA-C	-9.09	1.41	1.52
1	A	58	ARG	C-O	-9.03	1.13	1.24
1	B	111	ARG	C-O	-9.00	1.13	1.24
2	C	104	VAL	C-O	-9.00	1.13	1.24
1	A	51	ASP	C-O	-8.96	1.13	1.24
1	B	236	SER	CA-C	-8.86	1.41	1.52
1	B	234	THR	N-CA	-8.82	1.34	1.45
2	C	101	ASN	C-O	-8.82	1.13	1.24
2	C	60	ASP	C-O	-8.81	1.14	1.24
1	A	21	HIS	C-O	-8.81	1.13	1.23
1	A	114	LEU	N-CA	-8.77	1.35	1.46
1	A	66	GLU	C-O	-8.71	1.13	1.24
1	A	122	ASN	CA-C	-8.70	1.41	1.52
1	A	44	GLU	C-O	-8.65	1.13	1.24
1	B	123	GLU	C-O	-8.60	1.13	1.24
1	A	110	ASN	CG-ND2	-8.45	1.15	1.33
1	B	237	GLN	C-O	-8.39	1.14	1.24
2	D	113	GLU	N-CA	-8.35	1.36	1.46
2	C	63	LEU	C-O	-8.32	1.14	1.23
1	A	67	ARG	CA-C	-8.31	1.42	1.52
2	D	75	MET	CG-SD	-8.29	1.60	1.80
2	E	106	GLU	N-CA	-8.26	1.36	1.46
1	A	88	MET	C-O	-8.20	1.14	1.24
2	C	55	ARG	C-O	-8.20	1.13	1.23
1	A	75	LEU	N-CA	-8.18	1.36	1.46
1	A	71	GLN	N-CA	-8.16	1.36	1.46
2	C	61	LEU	C-O	-8.14	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	HIS	C-O	-8.09	1.13	1.23
2	D	123	ALA	C-O	-8.06	1.13	1.23
1	B	112	ARG	CA-C	-8.03	1.42	1.52
1	A	124	ARG	C-O	-8.00	1.14	1.24
1	A	29	LEU	CA-C	-7.97	1.42	1.52
1	A	131	SER	C-O	-7.97	1.13	1.23
1	A	110	ASN	CG-OD1	-7.95	1.08	1.23
1	A	52	GLY	C-O	-7.91	1.14	1.23
1	A	142	PHE	C-N	-7.87	1.23	1.33
1	B	155	ASP	N-CA	-7.87	1.36	1.46
2	D	109	GLU	C-N	-7.85	1.23	1.33
2	C	109	GLU	C-O	-7.84	1.14	1.24
1	A	127	ARG	C-O	-7.79	1.15	1.24
1	A	84	ARG	CA-CB	-7.78	1.41	1.53
2	E	41	GLN	C-O	-7.67	1.15	1.24
2	E	103	ARG	C-O	-7.66	1.15	1.24
1	B	239	VAL	C-O	-7.62	1.15	1.24
1	A	88	MET	N-CA	-7.57	1.37	1.46
1	A	47	ALA	N-CA	-7.53	1.37	1.46
2	C	110	GLU	C-O	-7.48	1.15	1.24
1	A	125	SER	CA-C	-7.46	1.43	1.52
1	B	117	ARG	C-O	-7.43	1.15	1.24
2	E	69	SER	CA-C	-7.41	1.43	1.52
1	A	68	TYR	N-CA	-7.39	1.37	1.46
1	A	111	ARG	CA-CB	-7.38	1.41	1.53
1	A	84	ARG	CA-C	-7.34	1.43	1.52
1	B	155	ASP	CA-C	-7.30	1.43	1.52
2	E	69	SER	C-O	-7.28	1.15	1.24
1	B	203	ARG	C-N	-7.26	1.24	1.33
2	D	110	GLU	N-CA	-7.26	1.37	1.46
1	A	23	HIS	CA-C	-7.25	1.44	1.53
2	D	113	GLU	C-O	-7.24	1.15	1.24
2	E	33	GLU	C-O	-7.24	1.15	1.23
1	A	116	GLU	N-CA	-7.24	1.37	1.46
1	A	125	SER	C-O	-7.22	1.15	1.24
2	D	10	GLN	CA-CB	-7.18	1.40	1.53
2	E	102	GLU	CA-C	-7.17	1.43	1.52
1	B	110	ASN	C-O	-7.17	1.14	1.23
2	C	105	ALA	N-CA	-7.17	1.37	1.46
2	C	54	GLN	C-O	-7.16	1.14	1.24
2	C	110	GLU	CA-C	-7.16	1.43	1.52
1	A	127	ARG	CA-C	-7.16	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	MET	CA-CB	-7.13	1.42	1.53
2	E	103	ARG	CA-C	-7.13	1.43	1.52
1	A	80	ARG	CA-C	-7.12	1.43	1.52
1	A	112	ARG	CZ-NH2	-7.11	1.24	1.33
2	D	75	MET	CA-CB	-7.10	1.42	1.53
1	A	73	ARG	N-CA	-7.06	1.37	1.46
1	A	111	ARG	NE-CZ	-7.00	1.25	1.33
1	A	115	LEU	N-CA	-6.98	1.37	1.46
1	A	23	HIS	C-N	-6.97	1.26	1.34
1	A	20	PHE	C-O	-6.92	1.14	1.24
1	B	110	ASN	CG-OD1	-6.92	1.10	1.23
1	A	71	GLN	CA-CB	-6.91	1.42	1.53
1	B	153	SER	N-CA	-6.87	1.38	1.46
1	B	236	SER	N-CA	-6.86	1.38	1.46
1	B	151	HIS	CA-C	-6.84	1.43	1.52
1	A	59	GLU	N-CA	-6.82	1.38	1.46
1	A	112	ARG	N-CA	-6.80	1.38	1.46
2	D	75	MET	CA-C	-6.76	1.44	1.52
1	B	230	ARG	C-O	-6.76	1.15	1.23
1	B	228	GLU	CA-C	-6.75	1.44	1.52
1	A	112	ARG	CA-C	-6.75	1.44	1.52
2	C	122	GLN	C-O	-6.75	1.16	1.24
1	B	238	THR	CB-CG2	-6.71	1.30	1.52
2	E	106	GLU	CA-CB	-6.70	1.43	1.53
2	E	33	GLU	N-CA	-6.69	1.37	1.46
1	B	149	TRP	N-CA	-6.68	1.37	1.46
2	E	105	ALA	C-O	-6.64	1.16	1.24
1	A	129	GLY	C-O	-6.63	1.15	1.23
2	C	121	ILE	C-O	-6.61	1.16	1.24
1	A	69	HIS	N-CA	-6.60	1.38	1.46
1	A	143	LYS	CA-CB	-6.57	1.43	1.53
1	A	109	PRO	CA-CB	-6.57	1.44	1.53
1	B	45	ARG	C-O	-6.56	1.16	1.24
2	E	82	GLU	C-O	-6.53	1.16	1.24
1	A	122	ASN	CG-ND2	-6.49	1.19	1.33
1	A	72	LEU	CA-C	-6.49	1.44	1.52
1	B	240	ASN	C-O	-6.45	1.16	1.24
1	A	113	MET	CA-CB	-6.44	1.43	1.53
1	B	112	ARG	CA-CB	-6.42	1.43	1.53
1	B	149	TRP	C-O	-6.42	1.15	1.24
2	C	123	ALA	C-O	-6.42	1.16	1.23
2	E	69	SER	N-CA	-6.41	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLN	N-CA	-6.40	1.38	1.46
2	D	124	HIS	C-O	-6.37	1.16	1.24
1	B	110	ASN	CG-ND2	-6.33	1.20	1.33
2	C	100	ARG	N-CA	-6.33	1.38	1.46
1	B	203	ARG	CZ-NH1	-6.28	1.24	1.32
1	B	229	HIS	C-O	-6.25	1.16	1.24
1	A	111	ARG	CA-C	-6.23	1.44	1.52
1	B	113	MET	C-O	-6.22	1.16	1.24
1	A	58	ARG	CA-C	-6.19	1.44	1.52
1	A	113	MET	N-CA	-6.16	1.39	1.46
1	B	112	ARG	CZ-NH2	-6.15	1.25	1.33
2	C	62	ARG	C-O	-6.11	1.14	1.23
1	A	131	SER	N-CA	-6.08	1.38	1.45
1	A	71	GLN	CA-C	-6.08	1.44	1.52
2	E	102	GLU	C-O	-6.07	1.17	1.24
1	A	80	ARG	CD-NE	-6.06	1.37	1.46
1	A	65	SER	C-N	-6.06	1.25	1.34
1	B	48	ARG	N-CA	-6.05	1.39	1.46
1	A	72	LEU	C-N	-6.05	1.25	1.33
1	A	87	GLN	C-N	-6.04	1.25	1.33
1	B	152	ASP	CA-C	-6.03	1.45	1.52
1	B	237	GLN	CA-C	-6.02	1.45	1.52
1	B	240	ASN	N-CA	-6.01	1.39	1.46
2	E	41	GLN	N-CA	-6.00	1.39	1.46
1	B	21	HIS	N-CA	-5.98	1.38	1.46
2	D	10	GLN	CA-C	-5.98	1.44	1.52
1	A	122	ASN	N-CA	-5.96	1.39	1.46
2	D	75	MET	N-CA	-5.95	1.39	1.46
1	A	49	ILE	CA-C	-5.94	1.45	1.52
1	B	203	ARG	CZ-NH2	-5.93	1.25	1.33
2	E	104	VAL	C-O	-5.93	1.17	1.24
1	B	236	SER	C-O	-5.93	1.17	1.24
1	A	48	ARG	N-CA	-5.92	1.39	1.46
1	A	58	ARG	N-CA	-5.91	1.39	1.46
1	B	237	GLN	N-CA	-5.91	1.39	1.46
1	B	150	GLY	CA-C	-5.91	1.45	1.52
1	B	117	ARG	C-N	-5.90	1.26	1.33
2	C	105	ALA	CA-C	-5.89	1.45	1.52
1	A	74	ARG	CZ-NH2	-5.87	1.25	1.33
1	B	238	THR	CA-CB	-5.87	1.44	1.53
2	E	41	GLN	CA-C	-5.87	1.45	1.52
2	C	102	GLU	C-O	-5.85	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	ASP	C-N	-5.84	1.26	1.33
2	C	123	ALA	CA-CB	-5.80	1.44	1.53
1	A	114	LEU	C-N	-5.78	1.26	1.33
1	A	109	PRO	N-CA	-5.78	1.40	1.47
1	A	72	LEU	N-CA	-5.77	1.39	1.46
1	A	66	GLU	N-CA	-5.75	1.39	1.46
2	C	63	LEU	CA-C	-5.75	1.45	1.52
1	A	50	SER	N-CA	-5.71	1.39	1.46
1	A	51	ASP	CG-OD1	-5.71	1.14	1.25
1	A	111	ARG	N-CA	-5.70	1.39	1.46
2	D	110	GLU	CD-OE1	-5.68	1.14	1.25
1	A	194	ASP	C-O	-5.67	1.16	1.24
1	B	158	LEU	CA-CB	-5.66	1.44	1.53
2	C	104	VAL	CA-CB	-5.64	1.47	1.54
1	A	22	GLY	C-O	-5.62	1.15	1.24
1	A	74	ARG	CA-C	-5.62	1.45	1.52
2	E	33	GLU	CA-C	-5.62	1.45	1.53
2	C	112	ARG	N-CA	-5.60	1.38	1.46
1	A	84	ARG	C-N	-5.59	1.26	1.33
1	A	25	LEU	CA-C	-5.58	1.44	1.52
1	B	156	ARG	CA-C	-5.57	1.45	1.52
2	D	123	ALA	CA-CB	-5.57	1.44	1.53
2	E	104	VAL	N-CA	-5.56	1.39	1.46
1	B	154	GLY	CA-C	-5.55	1.45	1.52
2	D	74	MET	C-N	-5.54	1.26	1.33
1	A	80	ARG	C-N	-5.54	1.26	1.33
1	B	233	GLU	C-N	-5.51	1.26	1.33
1	B	111	ARG	N-CA	-5.50	1.39	1.46
2	C	112	ARG	CA-CB	-5.50	1.43	1.53
2	C	112	ARG	CD-NE	-5.50	1.38	1.46
1	A	26	HIS	C-N	-5.49	1.26	1.34
1	A	128	HIS	CA-C	-5.49	1.45	1.52
2	D	110	GLU	CA-C	-5.49	1.45	1.52
1	B	233	GLU	CA-C	-5.48	1.45	1.53
1	A	44	GLU	CA-C	-5.47	1.45	1.52
1	B	239	VAL	CA-C	-5.46	1.45	1.52
2	C	103	ARG	N-CA	-5.44	1.38	1.46
2	C	58	GLU	N-CA	-5.43	1.39	1.46
1	A	28	ALA	N-CA	-5.41	1.39	1.46
1	A	80	ARG	CA-CB	-5.41	1.44	1.53
1	B	231	ILE	C-O	-5.38	1.18	1.24
1	B	238	THR	CA-C	-5.38	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	N-CA	-5.36	1.39	1.46
1	A	58	ARG	C-N	-5.36	1.27	1.33
1	B	144	GLN	N-CA	-5.36	1.39	1.46
1	A	67	ARG	C-N	-5.34	1.26	1.33
2	D	113	GLU	CA-CB	-5.33	1.45	1.53
1	A	46	ILE	N-CA	-5.32	1.40	1.46
1	A	88	MET	CA-C	-5.30	1.46	1.52
1	A	68	TYR	C-N	-5.29	1.26	1.33
1	A	47	ALA	CA-CB	-5.29	1.44	1.53
1	A	117	ARG	N-CA	-5.29	1.39	1.46
1	A	51	ASP	N-CA	-5.27	1.40	1.46
2	D	110	GLU	CD-OE2	-5.26	1.15	1.25
1	A	115	LEU	CA-CB	-5.26	1.45	1.53
1	B	111	ARG	CA-CB	-5.25	1.45	1.53
2	C	112	ARG	C-N	-5.24	1.27	1.33
1	A	29	LEU	N-CA	-5.24	1.40	1.46
1	B	149	TRP	CG-CD2	-5.24	1.34	1.43
1	A	66	GLU	C-N	-5.23	1.26	1.33
1	A	131	SER	CA-C	-5.22	1.45	1.53
2	D	10	GLN	C-N	-5.22	1.26	1.33
2	C	63	LEU	N-CA	-5.21	1.39	1.45
2	E	112	ARG	C-O	-5.20	1.17	1.24
2	C	123	ALA	CA-C	-5.20	1.46	1.52
2	D	112	ARG	C-N	-5.17	1.27	1.33
1	A	74	ARG	N-CA	-5.17	1.40	1.46
1	B	112	ARG	CZ-NH1	-5.17	1.25	1.32
1	B	229	HIS	CA-C	-5.13	1.46	1.52
1	B	117	ARG	CA-CB	-5.13	1.45	1.53
1	A	75	LEU	CA-C	-5.13	1.46	1.52
2	E	106	GLU	CA-C	-5.12	1.46	1.52
2	E	37	GLU	C-O	-5.11	1.18	1.24
1	B	228	GLU	C-O	-5.11	1.17	1.23
1	B	123	GLU	C-N	-5.10	1.26	1.33
1	B	240	ASN	CA-CB	-5.09	1.45	1.53
2	E	104	VAL	CA-CB	-5.08	1.48	1.54
1	A	73	ARG	CA-CB	-5.07	1.45	1.53
1	B	157	VAL	CA-C	-5.06	1.46	1.52
1	A	59	GLU	C-N	-5.05	1.27	1.33
1	A	111	ARG	CD-NE	-5.05	1.39	1.46
2	D	75	MET	SD-CE	-5.04	1.67	1.79
1	A	113	MET	C-N	-5.02	1.27	1.33
2	C	124	HIS	C-O	-5.01	1.17	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	40	GLY	CA-C-N	-9.72	107.22	120.44
2	E	40	GLY	C-N-CA	-9.72	107.22	120.44
1	B	231	ILE	N-CA-C	8.69	120.68	109.30
2	C	122	GLN	N-CA-C	8.66	122.55	108.34
2	C	61	LEU	N-CA-C	7.78	122.11	109.59
1	B	149	TRP	N-CA-C	7.56	122.51	113.28
1	A	127	ARG	N-CA-C	7.06	118.76	111.14
1	A	26	HIS	N-CA-C	6.51	118.17	111.14
2	C	102	GLU	N-CA-C	6.42	118.36	111.36
2	C	124	HIS	N-CA-CB	-6.22	101.19	110.71
1	A	110	ASN	N-CA-C	6.19	119.46	109.86
1	A	143	LYS	N-CA-CB	-6.09	101.17	110.12
2	C	101	ASN	N-CA-CB	6.02	119.58	109.94
1	B	152	ASP	CB-CG-OD2	5.86	131.87	118.40
1	B	233	GLU	CA-C-O	5.76	128.61	121.81
1	B	233	GLU	N-CA-CB	5.74	119.18	110.45
1	A	48	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	126	GLN	N-CA-CB	-5.55	101.96	110.01
2	D	124	HIS	N-CA-C	5.53	118.07	111.71
2	C	112	ARG	N-CA-C	5.49	119.97	113.16
1	A	48	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	E	105	ALA	CA-C-N	-5.38	113.44	120.44
2	E	105	ALA	C-N-CA	-5.38	113.44	120.44
1	B	230	ARG	CB-CG-CD	5.36	123.63	111.30
1	A	84	ARG	N-CA-C	5.35	117.11	111.28
1	A	88	MET	N-CA-CB	-5.33	102.27	110.16
2	C	112	ARG	N-CA-CB	-5.31	102.32	110.44
2	C	110	GLU	CB-CA-C	-5.21	101.17	110.70
1	B	112	ARG	CA-C-O	-5.19	115.37	120.82
2	E	106	GLU	CB-CA-C	-5.14	102.80	110.88
1	B	203	ARG	CA-C-O	5.13	125.85	120.42
2	E	69	SER	CB-CA-C	-5.12	102.28	110.79
2	C	62	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	A	114	LEU	CA-CB-CG	-5.03	98.70	116.30
2	D	110	GLU	N-CA-CB	-5.02	102.73	110.16
1	A	27	GLN	CA-C-N	5.00	126.98	120.28
1	A	27	GLN	C-N-CA	5.00	126.98	120.28

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	37	0
1	B	2103	0	2107	50	0
2	C	1007	0	949	26	0
2	D	1015	0	961	14	0
2	E	985	0	929	33	0
2	F	993	0	940	24	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	173	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 11.

All (173) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1:MET:HE2	1:A:5:ARG:NE	2.01	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:45:ARG:HG2	2:E:75:MET:HE1	1.75	0.68
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:E:106:GLU:O	2:E:107:LEU:C	2.39	0.62
2:F:92:SER:HB2	2:F:118:PRO:HB2	1.83	0.61
1:A:1:MET:HE2	1:A:5:ARG:HE	1.67	0.59
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:102:GLU:H	2:C:102:GLU:CD	2.08	0.58
2:C:23:ARG:HH11	2:C:23:ARG:HG3	1.69	0.58
2:D:15:ILE:HG12	2:D:26:MET:HG2	1.86	0.57
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:NH1	1:B:212:ARG:O	2.35	0.56
2:F:23:ARG:HH11	2:F:58:GLU:CD	2.14	0.56
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
2:E:41:GLN:O	2:E:42:VAL:C	2.47	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
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
1:B:46:ILE:HG12	2:E:75:MET:HE3	1.93	0.51
2:E:26:MET:HB3	2:E:63:LEU:HD21	1.93	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
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
2:E:40:GLY:O	2:E:41:GLN:C	2.50	0.49
1:A:133:VAL:HG22	1:A:187:LEU:HB2	1.95	0.49
2:D:26:MET:HE1	2:D:74:MET:HE1	1.93	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:B:191:ARG:HH11	1:B:228:GLU:CD	2.17	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1:MET:HB3	1:B:1:MET:HE2	1.43	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:C:23:ARG:HH12	2:C:58:GLU:CD	2.23	0.46
2:F:32:PRO:HD2	2:F:67:ASN:ND2	2.29	0.46
1:B:191:ARG:HD3	1:B:228:GLU:CD	2.36	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
1:B:191:ARG:NH1	1:B:228:GLU:CD	2.73	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
2:E:105:ALA:O	2:E:106:GLU:C	2.52	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
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:A:161:ILE:HG22	1:A:165:MET:HE2	1.99	0.44
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
1:B:136:MET:HE3	1:B:136:MET:HB3	1.92	0.43
1:A:192:LEU:HD12	1:A:192:LEU:HA	1.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:ARG:HD3	2:F:58:GLU:CD	2.43	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:A:138:ASP:OD1	1:A:250:LYS:NZ	2.51	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:E:19:TRP:NE1	2:E:55:ARG:HH22	2.18	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: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
1:B:74:ARG:HH22	2:C:79:ASP:CG	2.27	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
2:C:36:TYR:CD1	2:C:36:TYR:C	2.99	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
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
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
2:F:109:GLU:O	2:F:112:ARG:N	2.54	0.40
2:E:100:ARG:NH1	5:E:201:HOH:O	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	16	27
2	F	120/127 (94%)	114 (95%)	4 (3%)	2 (2%)	7	12
All	All	1004/1060 (95%)	970 (97%)	31 (3%)	3 (0%)	36	52

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%)	213 (94%)	14 (6%)	16	29
1	B	224/236 (95%)	215 (96%)	9 (4%)	28	47
2	C	107/110 (97%)	103 (96%)	4 (4%)	30	50
2	D	108/110 (98%)	105 (97%)	3 (3%)	38	60
2	E	104/110 (94%)	100 (96%)	4 (4%)	29	49
2	F	105/110 (96%)	105 (100%)	0	100	100
All	All	875/912 (96%)	841 (96%)	34 (4%)	28	48

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	33	ARG
1	A	58	ARG
1	A	71	GLN
1	A	90	ARG
1	A	113	MET
1	A	114	LEU
1	A	122	ASN
1	A	126	GLN
1	A	181	GLU
1	A	194	ASP
1	A	215	THR
1	A	247	LEU
1	A	250	LYS
1	B	1	MET
1	B	14	LEU
1	B	29	LEU
1	B	32	LEU
1	B	45	ARG
1	B	113	MET
1	B	123	GLU
1	B	152	ASP
1	B	174	LEU
2	C	54	GLN
2	C	102	GLU
2	C	103	ARG
2	C	122	GLN
2	D	58	GLU
2	D	75	MET
2	D	125	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	41	GLN
2	E	50	LEU
2	E	82	GLU
2	E	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	27	GLN
1	A	34	GLN
1	A	151	HIS
1	A	193	GLN
1	B	19	GLN
1	B	27	GLN
1	B	71	GLN
1	B	93	ASN
1	B	144	GLN
1	B	189	GLN
2	C	5	HIS
2	C	124	HIS
2	D	5	HIS
2	F	122	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	30,34,34	4.29	20 (66%)	46,54,54	2.69	20 (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	-	4/19/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	G2P	PB-O1B	-10.70	1.30	1.56
4	A	302	G2P	PB-O2B	-7.64	1.33	1.51
4	A	302	G2P	PA-O1A	-6.93	1.39	1.56
4	A	302	G2P	PG-O2G	-6.41	1.30	1.50
4	A	302	G2P	PG-O1G	-6.32	1.31	1.54
4	A	302	G2P	C5-N7	-6.26	1.26	1.39
4	A	302	G2P	O4'-C4'	-5.97	1.31	1.45
4	A	302	G2P	PG-O3G	-5.68	1.33	1.54
4	A	302	G2P	C2-N2	-4.70	1.23	1.34
4	A	302	G2P	O4'-C1'	-4.18	1.32	1.42
4	A	302	G2P	C3'-C4'	-3.62	1.43	1.53
4	A	302	G2P	C5-C6	-3.60	1.31	1.44
4	A	302	G2P	C2'-C1'	-3.56	1.42	1.53
4	A	302	G2P	C8-N9	-3.55	1.29	1.37
4	A	302	G2P	C4-N9	-3.43	1.29	1.38
4	A	302	G2P	PA-O2A	-3.02	1.44	1.51
4	A	302	G2P	O2'-C2'	-2.39	1.37	1.43
4	A	302	G2P	O6-C6	-2.22	1.19	1.23
4	A	302	G2P	O3'-C3'	-2.09	1.37	1.43
4	A	302	G2P	C1'-N9	-2.01	1.41	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	G2P	O4'-C1'-C2'	-7.03	91.57	106.62
4	A	302	G2P	O2A-PA-C3A	-6.68	91.45	109.05
4	A	302	G2P	O1A-PA-C3A	-5.87	82.42	106.73
4	A	302	G2P	C5-C4-N3	-5.67	119.37	128.39
4	A	302	G2P	C2-N3-C4	5.15	121.17	112.30
4	A	302	G2P	O1A-PA-O2A	3.98	122.89	109.95
4	A	302	G2P	C2-N1-C6	-3.63	118.53	125.11
4	A	302	G2P	O4'-C4'-C3'	-3.36	98.47	105.15
4	A	302	G2P	C1'-N9-C4	3.13	135.72	126.49
4	A	302	G2P	C4-C5-N7	-2.69	106.41	110.67
4	A	302	G2P	PB-O3B-PG	2.69	142.07	132.45
4	A	302	G2P	C1'-N9-C8	-2.52	119.56	126.73
4	A	302	G2P	O4'-C4'-C5'	-2.46	101.45	109.33
4	A	302	G2P	C5-C4-N9	2.44	110.02	105.66
4	A	302	G2P	O2B-PB-C3A	-2.43	102.65	109.05
4	A	302	G2P	N9-C4-N3	2.32	130.59	125.95
4	A	302	G2P	C8-N7-C5	2.28	108.31	104.26
4	A	302	G2P	C4'-O4'-C1'	-2.20	104.62	109.47
4	A	302	G2P	C5-C6-N1	2.18	118.79	113.25
4	A	302	G2P	C6-C5-C4	2.12	122.02	118.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	G2P	PB-C3A-PA-O1A
4	A	302	G2P	PB-C3A-PA-O2A
4	A	302	G2P	PB-C3A-PA-O5'
4	A	302	G2P	O4'-C4'-C5'-O5'

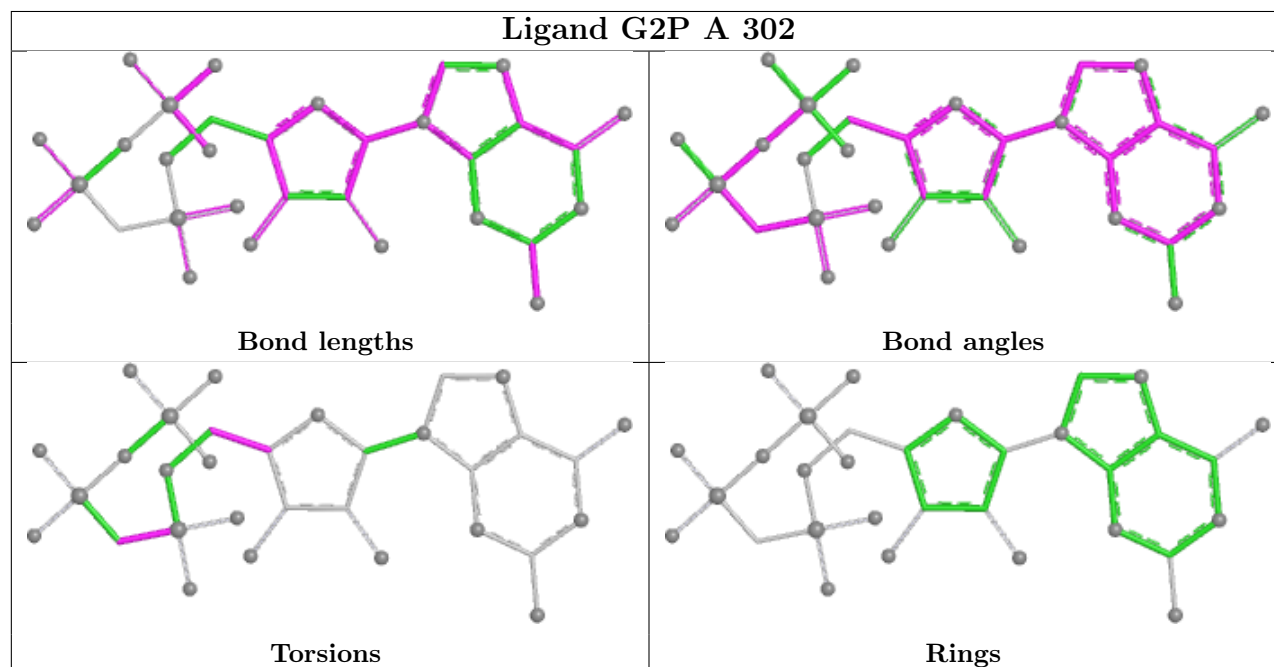
There are no ring outliers.

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%)	0.11	10 (3%) 44 36	19, 42, 70, 115	0
1	B	260/276 (94%)	0.30	7 (2%) 56 49	23, 50, 78, 102	0
2	C	124/127 (97%)	0.35	5 (4%) 42 34	26, 51, 80, 102	0
2	D	125/127 (98%)	-0.40	1 (0%) 82 79	16, 27, 54, 69	0
2	E	121/127 (95%)	1.74	43 (35%) 1 0	51, 96, 127, 131	0
2	F	122/127 (96%)	1.23	20 (16%) 4 3	41, 74, 102, 108	0
All	All	1016/1060 (95%)	0.45	86 (8%) 16 12	16, 50, 102, 131	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	19	TRP	4.9
1	A	264	PRO	4.9
1	A	262	LEU	4.7
2	E	50	LEU	4.2
1	A	261	ALA	4.1
2	E	91	VAL	3.8
2	E	49	PHE	3.7
2	E	95	TRP	3.7
2	F	90	PRO	3.6
2	F	49	PHE	3.6
2	F	116	SER	3.5
2	F	88	GLY	3.5
1	A	263	PRO	3.5
2	E	88	GLY	3.4
2	E	54	GLN	3.4
2	E	57	LEU	3.3
2	E	51	ALA	3.3
2	E	59	LEU	3.2
2	E	65	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	19	TRP	3.2
2	C	54	GLN	3.1
2	E	71	ILE	3.1
1	A	260	ALA	3.1
2	E	45	TRP	3.0
2	E	64	LEU	2.9
1	A	21	HIS	2.9
2	F	110	GLU	2.9
2	E	123	ALA	2.9
2	E	56	PRO	2.9
2	F	21	ALA	2.9
2	F	81	LEU	2.8
2	E	124	HIS	2.8
2	F	117	PHE	2.8
2	E	90	PRO	2.8
1	A	130	GLN	2.8
2	C	125	ASP	2.8
2	E	119	PHE	2.8
2	C	99	ARG	2.8
2	E	66	LEU	2.7
2	E	53	GLY	2.7
1	A	191	ARG	2.7
2	F	18	ASP	2.7
2	D	101	ASN	2.6
2	E	46	VAL	2.6
1	B	130	GLN	2.6
1	B	101	ILE	2.6
2	E	55	ARG	2.6
2	F	51	ALA	2.6
2	E	111	PHE	2.5
1	B	230	ARG	2.5
2	E	38	LEU	2.5
2	E	36	TYR	2.5
2	F	56	PRO	2.5
2	F	54	GLN	2.5
2	E	120	ALA	2.5
2	E	61	LEU	2.4
2	F	50	LEU	2.4
2	F	59	LEU	2.4
2	E	117	PHE	2.4
2	C	98	ASP	2.4
2	E	94	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	128	HIS	2.4
1	A	2	SER	2.3
2	E	60	ASP	2.2
2	F	45	TRP	2.2
2	F	57	LEU	2.2
2	E	6	ILE	2.2
1	B	192	LEU	2.2
2	E	92	SER	2.2
2	E	20	GLN	2.2
2	E	23	ARG	2.1
1	B	193	GLN	2.1
2	E	74	MET	2.1
2	E	43	ILE	2.1
2	F	3	ASP	2.1
2	F	91	VAL	2.1
2	E	96	HIS	2.1
2	C	102	GLU	2.1
2	E	89	ARG	2.1
2	E	125	ASP	2.0
2	F	48	ARG	2.0
2	E	87	GLY	2.0
1	A	4	GLU	2.0
2	E	63	LEU	2.0
1	B	231	ILE	2.0
2	E	121	ILE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

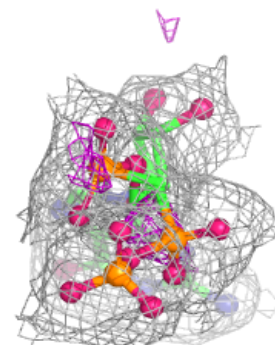
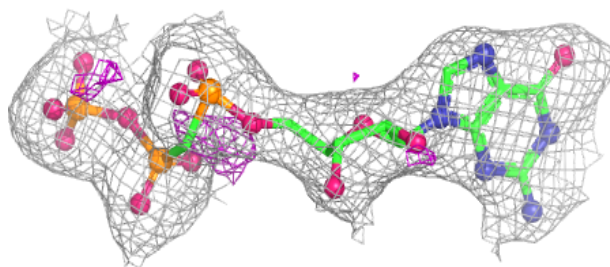
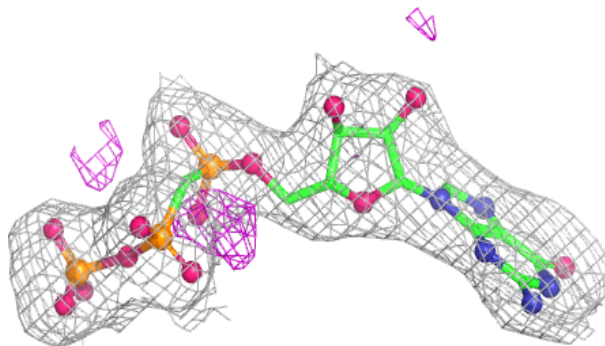
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	G2P	A	302	32/32	0.93	0.08	35,51,68,99	0
3	MG	A	301	1/1	0.98	0.07	28,28,28,28	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.

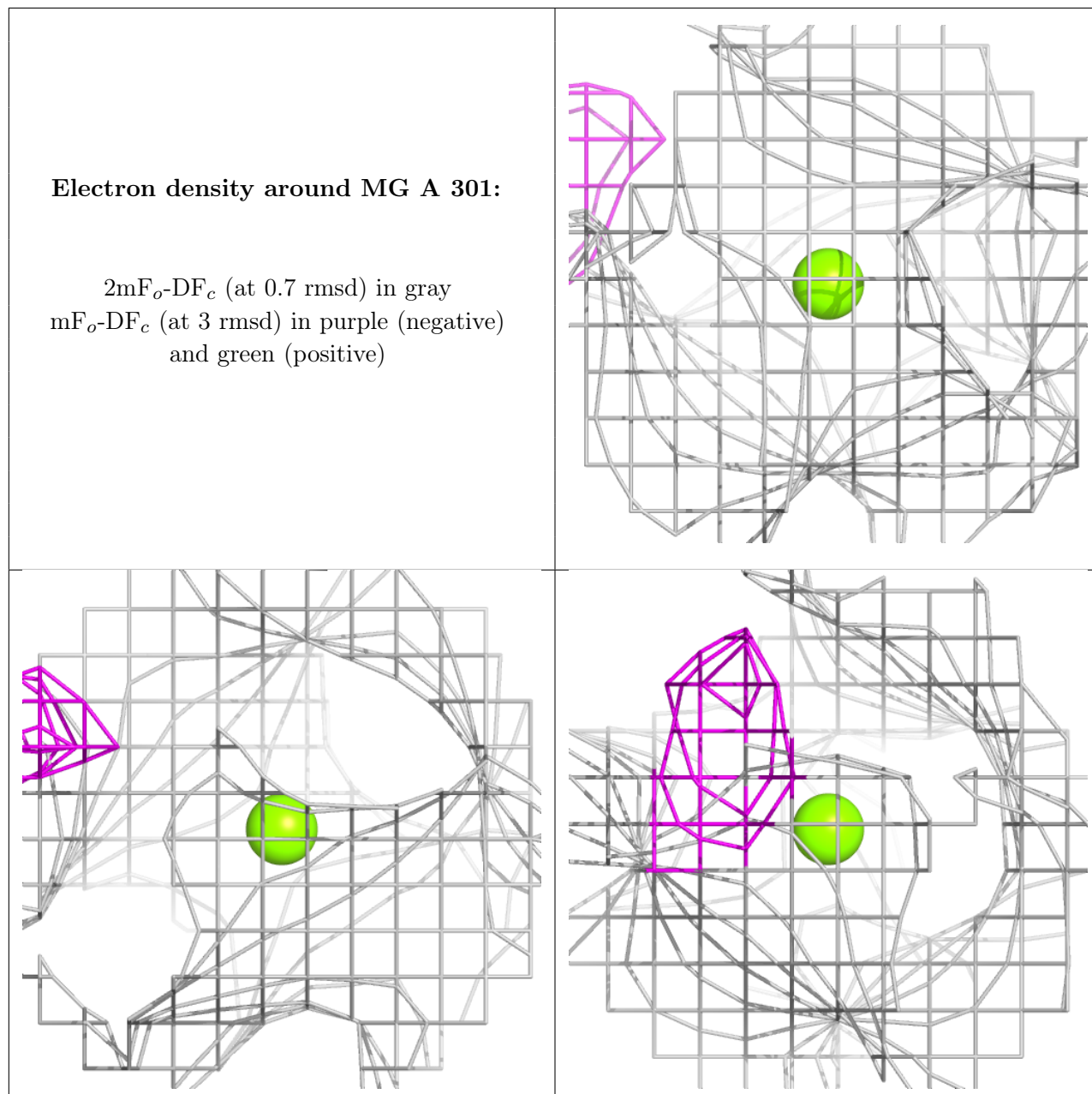
Electron density around G2P A 302:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.