



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:20 pm BST

PDB ID : 2AZ3
Title : Structure of a halophilic nucleoside diphosphate kinase from Halobacterium salinarum in complex with CDP
Authors : Besir, H.; Zeth, K.; Bracher, A.; Heider, U.; Ishibashi, M.; Tokunaga, M.; Oesterhelt, D.
Deposited on : 2005-09-09
Resolution : 2.20 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

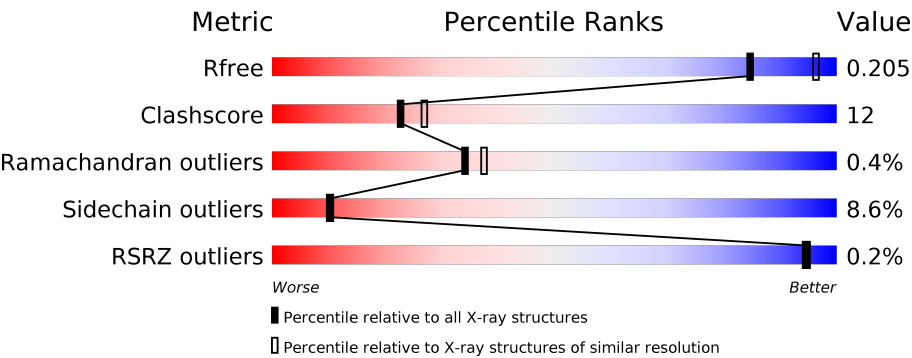
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	164	<div><div>%</div><div><div></div><div>66%</div><div>22%</div><div>•</div><div>7%</div></div></div>
1	B	164	<div><div></div><div>66%</div><div>23%</div><div>•</div><div>8%</div></div>
1	C	164	<div><div></div><div>67%</div><div>21%</div><div>5%</div><div>7%</div></div>
1	D	164	<div><div></div><div>70%</div><div>18%</div><div>5%</div><div>7%</div></div>
1	E	164	<div><div></div><div>68%</div><div>20%</div><div>5%</div><div>7%</div></div>
1	F	164	<div><div>%</div><div><div></div><div>54%</div><div>34%</div><div>• •</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	164	<div><div>%</div><div><div></div><div>60%</div><div>28%</div><div>•</div><div>7%</div></div></div>
1	H	164	<div><div></div><div>66%</div><div>20%</div><div>7%</div><div>7%</div></div>
1	I	164	<div><div></div><div>63%</div><div>26%</div><div>•</div><div>8%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11117 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1188	741	205	237	5			
1	B	151	Total	C	N	O	S	0	0	0
			1191	743	205	238	5			
1	C	153	Total	C	N	O	S	0	0	0
			1206	752	209	240	5			
1	D	152	Total	C	N	O	S	0	0	0
			1192	744	206	237	5			
1	E	152	Total	C	N	O	S	0	0	0
			1188	742	206	235	5			
1	F	152	Total	C	N	O	S	0	0	0
			1201	749	208	239	5			
1	G	152	Total	C	N	O	S	0	1	0
			1206	753	212	236	5			
1	H	152	Total	C	N	O	S	0	1	0
			1195	745	209	236	5			
1	I	151	Total	C	N	O	S	0	0	0
			1183	739	205	234	5			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P61136
A	-1	SER	-	CLONING ARTIFACT	UNP P61136
A	0	HIS	-	CLONING ARTIFACT	UNP P61136
B	-2	GLY	-	CLONING ARTIFACT	UNP P61136
B	-1	SER	-	CLONING ARTIFACT	UNP P61136
B	0	HIS	-	CLONING ARTIFACT	UNP P61136
C	-2	GLY	-	CLONING ARTIFACT	UNP P61136
C	-1	SER	-	CLONING ARTIFACT	UNP P61136
C	0	HIS	-	CLONING ARTIFACT	UNP P61136
D	-2	GLY	-	CLONING ARTIFACT	UNP P61136
D	-1	SER	-	CLONING ARTIFACT	UNP P61136

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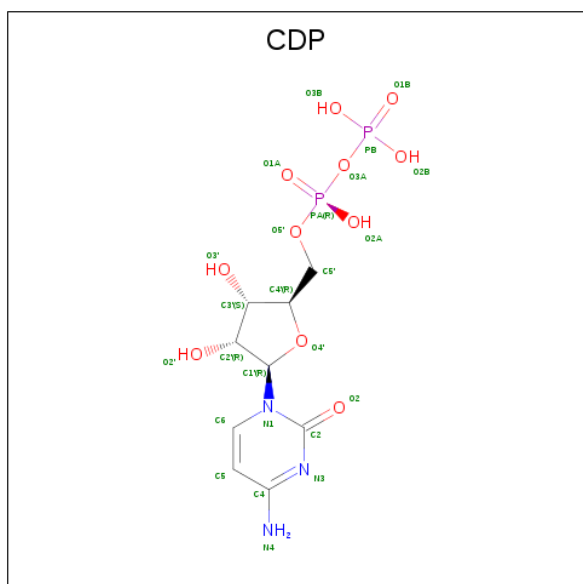
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	CLONING ARTIFACT	UNP P61136
E	-2	GLY	-	CLONING ARTIFACT	UNP P61136
E	-1	SER	-	CLONING ARTIFACT	UNP P61136
E	0	HIS	-	CLONING ARTIFACT	UNP P61136
F	-2	GLY	-	CLONING ARTIFACT	UNP P61136
F	-1	SER	-	CLONING ARTIFACT	UNP P61136
F	0	HIS	-	CLONING ARTIFACT	UNP P61136
G	-2	GLY	-	CLONING ARTIFACT	UNP P61136
G	-1	SER	-	CLONING ARTIFACT	UNP P61136
G	0	HIS	-	CLONING ARTIFACT	UNP P61136
H	-2	GLY	-	CLONING ARTIFACT	UNP P61136
H	-1	SER	-	CLONING ARTIFACT	UNP P61136
H	0	HIS	-	CLONING ARTIFACT	UNP P61136
I	-2	GLY	-	CLONING ARTIFACT	UNP P61136
I	-1	SER	-	CLONING ARTIFACT	UNP P61136
I	0	HIS	-	CLONING ARTIFACT	UNP P61136

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: C₉H₁₅N₃O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	E	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	F	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	G	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	H	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	I	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

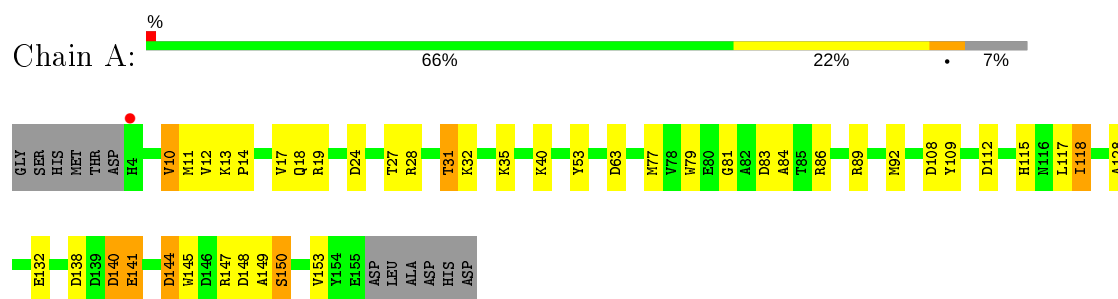
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	19	Total	O	0	0
			19	19		
4	C	19	Total	O	0	0
			19	19		
4	D	15	Total	O	0	0
			15	15		
4	E	12	Total	O	0	0
			12	12		
4	F	13	Total	O	0	0
			13	13		
4	G	11	Total	O	0	0
			11	11		
4	H	17	Total	O	0	0
			17	17		
4	I	9	Total	O	0	0
			9	9		

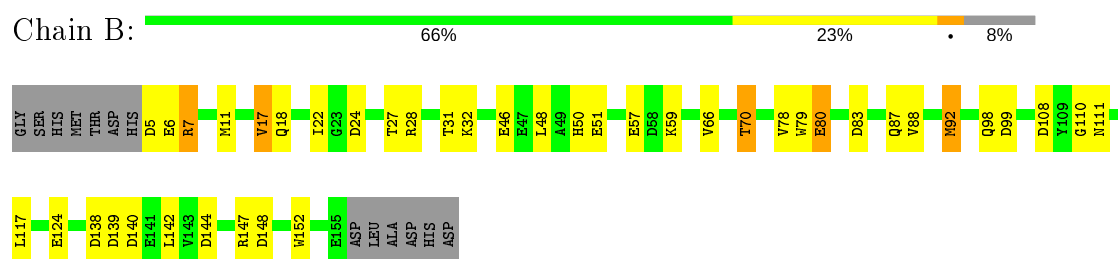
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

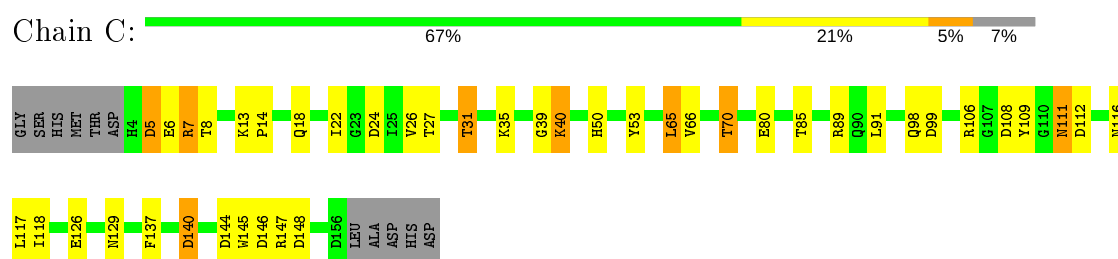
- Molecule 1: Nucleoside diphosphate kinase



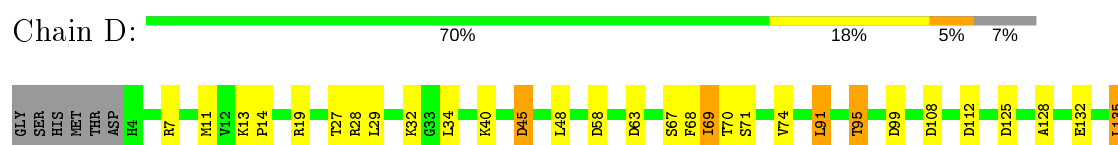
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase





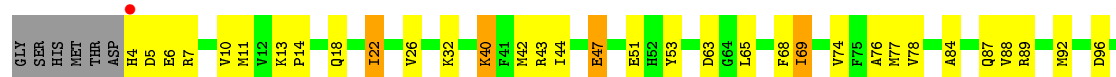
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase

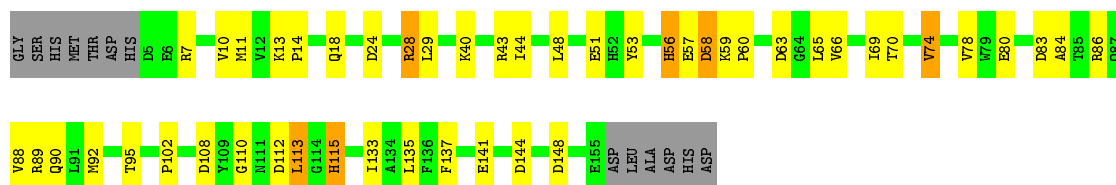


- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.37Å 71.52Å 157.99Å 90.00° 95.53° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 157.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	80.4 (20.00-2.20) 80.3 (157.25-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.200 , 0.271 0.206 , 0.205	Depositor DCC
R_{free} test set	2853 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11117	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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, CDP

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	1.12	4/1214 (0.3%)	1.21	11/1643 (0.7%)
1	B	1.10	3/1217 (0.2%)	1.30	15/1645 (0.9%)
1	C	1.07	1/1233 (0.1%)	1.14	8/1667 (0.5%)
1	D	0.95	0/1218	1.15	13/1647 (0.8%)
1	E	0.94	0/1214	1.16	10/1642 (0.6%)
1	F	0.97	0/1228	1.19	14/1660 (0.8%)
1	G	0.92	1/1233 (0.1%)	1.12	11/1666 (0.7%)
1	H	0.90	0/1221	1.10	7/1652 (0.4%)
1	I	0.96	0/1209	1.09	5/1635 (0.3%)
All	All	1.00	9/10987 (0.1%)	1.16	94/14857 (0.6%)

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	B	0	1
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	MET	SD-CE	-6.82	1.39	1.77
1	A	12	VAL	CB-CG2	6.35	1.66	1.52
1	B	5	ASP	CB-CG	6.22	1.64	1.51
1	B	17	VAL	CB-CG2	-6.04	1.40	1.52
1	C	111	ASN	CB-CG	-5.79	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	TYR	CD2-CE2	5.70	1.47	1.39
1	G	76	ALA	CA-CB	-5.69	1.40	1.52
1	A	109	TYR	CD2-CE2	5.45	1.47	1.39
1	A	17	VAL	CB-CG2	-5.19	1.42	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	24	ASP	CB-CG-OD2	9.56	126.90	118.30
1	D	140	ASP	CB-CG-OD2	9.21	126.58	118.30
1	E	148	ASP	CB-CG-OD2	9.00	126.40	118.30
1	C	140	ASP	CB-CG-OD2	8.72	126.15	118.30
1	A	148	ASP	CB-CG-OD2	8.72	126.15	118.30
1	B	5	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	108	ASP	CB-CG-OD2	8.65	126.08	118.30
1	D	99	ASP	CB-CG-OD2	8.64	126.07	118.30
1	B	148	ASP	CB-CG-OD2	8.60	126.04	118.30
1	A	140	ASP	CB-CG-OD2	8.55	125.99	118.30
1	G	108	ASP	CB-CG-OD2	8.45	125.90	118.30
1	E	96	ASP	CB-CG-OD2	8.31	125.78	118.30
1	F	108	ASP	CB-CG-OD2	8.25	125.72	118.30
1	B	147	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	5	ASP	CB-CG-OD2	8.12	125.60	118.30
1	B	140	ASP	CB-CG-OD2	7.86	125.38	118.30
1	C	148	ASP	CB-CG-OD2	7.76	125.28	118.30
1	C	108	ASP	CB-CG-OD2	7.62	125.16	118.30
1	I	63	ASP	CB-CG-OD2	7.62	125.16	118.30
1	B	28	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	24	ASP	CB-CG-OD2	7.51	125.06	118.30
1	F	148	ASP	CB-CG-OD2	7.49	125.04	118.30
1	B	108	ASP	CB-CG-OD2	7.48	125.03	118.30
1	G	96	ASP	CB-CG-OD2	7.35	124.92	118.30
1	H	146	ASP	CB-CG-OD2	7.24	124.82	118.30
1	C	99	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	147	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	15	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	28	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	144	ASP	CB-CG-OD2	7.02	124.62	118.30
1	G	125	ASP	CB-CG-OD2	6.93	124.54	118.30
1	D	148	ASP	CB-CG-OD2	6.87	124.48	118.30
1	F	122	ASP	CB-CG-OD2	6.73	124.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	139	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	138	ASP	CB-CG-OD2	6.63	124.27	118.30
1	E	99	ASP	CB-CG-OD2	6.62	124.25	118.30
1	H	83	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	83	ASP	CB-CG-OD2	6.54	124.19	118.30
1	D	58	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	99	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	112	ASP	CB-CG-OD2	6.36	124.03	118.30
1	H	144	ASP	CB-CG-OD2	6.33	124.00	118.30
1	D	139	ASP	CB-CG-OD1	6.28	123.95	118.30
1	I	28	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	F	45	ASP	CB-CG-OD2	6.22	123.90	118.30
1	D	63	ASP	CB-CG-OD2	6.18	123.86	118.30
1	H	58	ASP	CB-CG-OD2	6.15	123.83	118.30
1	G	146	ASP	CB-CG-OD2	6.14	123.83	118.30
1	I	24	ASP	CB-CG-OD2	6.00	123.70	118.30
1	H	148	ASP	CB-CG-OD2	5.98	123.68	118.30
1	F	63	ASP	CB-CG-OD2	5.97	123.68	118.30
1	E	28	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	D	108	ASP	CB-CG-OD2	5.94	123.64	118.30
1	F	96	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	5	ASP	OD1-CG-OD2	-5.84	112.21	123.30
1	B	144	ASP	CB-CG-OD1	5.82	123.54	118.30
1	H	108	ASP	CB-CG-OD2	5.82	123.53	118.30
1	E	112	ASP	CB-CG-OD2	5.81	123.53	118.30
1	F	89	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	G	63	ASP	CB-CG-OD2	5.74	123.47	118.30
1	I	144	ASP	CB-CG-OD2	5.73	123.46	118.30
1	G	148	ASP	CB-CG-OD2	5.73	123.45	118.30
1	F	58	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	125	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	45	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	24	ASP	CB-CG-OD2	5.67	123.41	118.30
1	F	24	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	112	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	28	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	I	108	ASP	CB-CG-OD2	5.57	123.31	118.30
1	G	99	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	19	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	F	112	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	28	ARG	NE-CZ-NH1	5.45	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	5	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	125	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	138	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	112	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	144	ASP	CB-CG-OD2	5.41	123.17	118.30
1	E	138	ASP	CB-CG-OD2	5.38	123.15	118.30
1	G	89	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	F	138	ASP	CB-CG-OD2	5.34	123.11	118.30
1	H	99	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	140	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	58	ASP	CB-CG-OD2	5.27	123.04	118.30
1	G	112	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	125	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	144	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	63	ASP	CB-CG-OD1	5.14	122.93	118.30
1	E	117	LEU	CA-CB-CG	5.07	126.97	115.30
1	C	146	ASP	CB-CG-OD1	5.07	122.86	118.30
1	G	139	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	GLY	Peptide
1	E	116	ASN	Peptide
1	G	110	GLY	Peptide
1	H	116	ASN	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	1188	0	1090	22	0
1	B	1191	0	1103	17	0
1	C	1206	0	1112	35	0
1	D	1192	0	1101	24	0
1	E	1188	0	1097	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1201	0	1110	42	0
1	G	1206	0	1118	43	0
1	H	1195	0	1098	28	0
1	I	1183	0	1095	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	12	0	0
3	B	25	0	12	0	0
3	C	25	0	12	3	0
3	D	25	0	12	2	0
3	E	25	0	12	2	0
3	F	25	0	12	0	0
3	G	25	0	12	1	0
3	H	25	0	12	0	0
3	I	25	0	12	0	0
4	A	25	0	0	0	0
4	B	19	0	0	1	0
4	C	19	0	0	3	0
4	D	15	0	0	1	0
4	E	12	0	0	0	0
4	F	13	0	0	1	0
4	G	11	0	0	0	0
4	H	17	0	0	0	0
4	I	9	0	0	0	0
All	All	11117	0	10032	242	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 12.

All (242) 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:G:40:LYS:NZ	1:G:141:GLU:OE2	2.00	0.94
1:I:11:MET:CE	1:I:69:ILE:HD11	1.99	0.92
1:F:148:ASP:H	1:G:18:GLN:HE22	1.16	0.91
1:F:148:ASP:H	1:G:18:GLN:NE2	1.67	0.91
1:C:98:GLN:HG2	1:C:111:ASN:HB2	1.56	0.86
1:C:40:LYS:HD2	1:C:137:PHE:HE1	1.42	0.85
1:A:128:ALA:O	1:A:132:GLU:HG3	1.78	0.83
1:E:110:GLY:O	1:F:32:LYS:HE2	1.77	0.82
1:I:135:LEU:HD23	1:I:135:LEU:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:TRP:CE2	1:F:18:GLN:HG2	2.17	0.79
1:C:85:THR:HG21	1:C:129:ASN:HD22	1.48	0.79
1:H:11:MET:HE1	1:H:44:ILE:HD11	1.65	0.78
1:I:53:TYR:CD2	1:I:65:LEU:HD21	2.17	0.78
1:D:148:ASP:H	1:I:18:GLN:NE2	1.82	0.78
1:C:40:LYS:HD2	1:C:137:PHE:CE1	2.20	0.76
1:E:27:THR:O	1:E:31:THR:HG23	1.86	0.76
1:B:7:ARG:NH1	1:B:80:GLU:OE1	2.20	0.74
1:G:152:TRP:CE2	1:I:18:GLN:HG2	2.24	0.73
1:I:40:LYS:NZ	1:I:141:GLU:OE1	2.22	0.72
1:G:18:GLN:HG2	1:H:152:TRP:CE2	2.25	0.71
1:H:35:LYS:NZ	1:H:80:GLU:OE2	2.24	0.70
1:D:32:LYS:O	1:D:32:LYS:HG3	1.92	0.69
1:G:145:TRP:CH2	1:G:147[B]:ARG:HG2	2.28	0.69
1:G:13:LYS:HB3	1:G:14:PRO:CD	2.23	0.69
1:C:40:LYS:CD	1:C:137:PHE:CE1	2.76	0.68
1:C:109:TYR:HB2	1:C:117:LEU:HD21	1.75	0.68
1:C:40:LYS:CD	1:C:137:PHE:HE1	2.06	0.67
1:H:67:SER:O	1:H:70:THR:HG22	1.92	0.67
1:C:109:TYR:CB	1:C:117:LEU:HD21	2.25	0.66
1:C:65:LEU:HD11	3:C:1300:CDP:O4'	1.94	0.66
1:C:6:GLU:OE2	1:C:85:THR:HG23	1.95	0.66
1:E:110:GLY:O	1:F:32:LYS:CE	2.44	0.65
1:F:44:ILE:O	1:F:70:THR:HG22	1.97	0.65
1:E:113:LEU:HD21	3:E:1500:CDP:N3	2.12	0.65
1:E:18:GLN:NE2	1:H:146:ASP:O	2.31	0.64
1:G:53:TYR:CZ	1:G:65:LEU:HD22	2.34	0.63
1:C:8:THR:HB	1:C:85:THR:HG22	1.79	0.62
1:C:39:GLY:H	1:C:40:LYS:NZ	1.97	0.62
1:G:155:GLU:HG2	1:I:112:ASP:OD2	1.98	0.62
1:A:10:VAL:HG13	1:A:79:TRP:HD1	1.65	0.62
1:H:6:GLU:O	1:H:80:GLU:HA	1.99	0.62
1:I:7:ARG:NH1	1:I:80:GLU:OE1	2.33	0.61
1:I:11:MET:HE1	1:I:69:ILE:HD11	1.82	0.61
1:E:66:VAL:O	1:E:70:THR:HB	1.99	0.61
1:C:109:TYR:HB2	1:C:117:LEU:CD2	2.31	0.61
1:F:148:ASP:N	1:G:18:GLN:HE22	1.92	0.61
1:H:86[B]:ARG:NH1	1:H:90:GLN:HE22	1.99	0.61
1:E:95:THR:HA	1:E:106:ARG:NH1	2.16	0.60
1:D:29:LEU:HD23	1:D:91:LEU:HD23	1.83	0.60
1:C:65:LEU:HD11	3:C:1300:CDP:C1'	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:THR:O	1:C:31:THR:HB	2.02	0.59
1:G:40:LYS:HE3	1:G:42:MET:HE2	1.84	0.59
1:I:133:ILE:O	1:I:137:PHE:HB2	2.02	0.59
1:E:17:VAL:HG22	1:E:22:ILE:HD11	1.84	0.59
1:F:88:VAL:O	1:F:92:MET:HG3	2.01	0.58
1:G:68:PHE:CD1	1:G:115:HIS:CE1	2.92	0.57
1:G:88:VAL:O	1:G:92:MET:HG3	2.04	0.57
1:D:152:TRP:NE1	1:F:18:GLN:HG2	2.20	0.57
1:F:13:LYS:NZ	1:F:119:HIS:HB2	2.20	0.57
1:G:13:LYS:HB3	1:G:14:PRO:HD2	1.86	0.56
1:E:115:HIS:CD2	1:F:155:GLU:HG2	2.41	0.56
1:F:95:THR:HG23	4:F:1610:HOH:O	2.05	0.56
1:I:11:MET:HE2	1:I:69:ILE:HD11	1.86	0.56
1:A:89:ARG:HA	1:A:92:MET:HE2	1.88	0.56
1:B:46:GLU:O	1:B:50:HIS:HD2	1.89	0.56
1:B:111:ASN:OD1	1:B:111:ASN:N	2.37	0.55
1:E:88:VAL:HG23	1:E:92:MET:HE2	1.88	0.55
1:E:9:PHE:CZ	1:E:11:MET:HE3	2.42	0.55
1:H:7:ARG:NH1	1:H:80:GLU:OE1	2.40	0.55
1:C:66:VAL:HG21	4:C:1304:HOH:O	2.06	0.55
1:D:95:THR:HG21	3:D:1400:CDP:PB	2.47	0.54
1:I:59:LYS:HB3	1:I:60:PRO:HD2	1.88	0.54
1:E:88:VAL:HG23	1:E:92:MET:CE	2.38	0.54
1:G:40:LYS:HE3	1:G:42:MET:CE	2.37	0.54
1:D:19:ARG:NH1	1:E:153:VAL:HG22	2.23	0.54
1:C:85:THR:HG21	1:C:129:ASN:ND2	2.20	0.54
1:C:53:TYR:CE2	1:C:65:LEU:HD23	2.42	0.54
1:A:35:LYS:HG3	1:A:145:TRP:CZ2	2.44	0.53
1:A:27:THR:O	1:A:31:THR:HB	2.08	0.53
1:D:148:ASP:H	1:I:18:GLN:HE21	1.55	0.53
1:G:152:TRP:CD2	1:I:18:GLN:HG2	2.43	0.53
1:G:40:LYS:CE	1:G:42:MET:HE2	2.39	0.53
1:G:11:MET:HE1	1:G:69:ILE:HD11	1.90	0.53
1:C:13:LYS:HB3	1:C:14:PRO:CD	2.39	0.53
1:C:40:LYS:HD3	1:C:137:PHE:CE1	2.44	0.53
1:C:66:VAL:O	1:C:70:THR:HB	2.08	0.53
1:I:113:LEU:HD23	1:I:113:LEU:O	2.10	0.52
1:A:117:LEU:C	1:A:118:ILE:HG22	2.28	0.52
1:G:152:TRP:O	1:I:115:HIS:HD2	1.92	0.52
1:D:147:ARG:O	1:D:150:SER:HB2	2.10	0.52
1:G:22:ILE:O	1:G:26:VAL:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:LEU:HD11	3:G:1700:CDP:O4'	2.09	0.51
1:B:98:GLN:HG2	1:B:111:ASN:HB2	1.93	0.51
1:B:7:ARG:CG	1:B:7:ARG:HH11	2.23	0.51
1:G:145:TRP:CZ3	1:G:147[B]:ARG:HG2	2.44	0.51
1:F:17:VAL:HG23	1:F:18:GLN:N	2.24	0.51
1:I:53:TYR:CE2	1:I:65:LEU:HD21	2.46	0.51
1:D:48:LEU:HD12	1:D:48:LEU:O	2.11	0.50
1:D:48:LEU:CD1	1:D:135:LEU:HD22	2.41	0.50
1:G:40:LYS:CE	1:G:42:MET:CE	2.90	0.50
1:H:35:LYS:HE3	1:H:145:TRP:O	2.11	0.50
1:F:67:SER:O	1:F:71:SER:HB3	2.12	0.50
1:B:88:VAL:HG12	1:B:92:MET:HE3	1.94	0.50
1:E:9:PHE:HZ	1:E:11:MET:HE3	1.76	0.50
1:B:32:LYS:NZ	1:B:87:GLN:OE1	2.33	0.50
1:E:11:MET:HE1	1:E:44:ILE:HD11	1.92	0.50
1:I:88:VAL:O	1:I:92:MET:HG3	2.12	0.50
1:A:83:ASP:OD2	1:A:86:ARG:HD3	2.12	0.50
1:D:147:ARG:HA	1:I:18:GLN:HE22	1.77	0.50
1:D:152:TRP:CD1	1:F:18:GLN:HG2	2.48	0.49
1:D:152:TRP:CD2	1:F:18:GLN:HG2	2.47	0.49
1:G:18:GLN:HG2	1:H:152:TRP:CD2	2.48	0.49
1:B:66:VAL:O	1:B:70:THR:HB	2.13	0.49
1:C:39:GLY:H	1:C:40:LYS:HZ2	1.61	0.49
1:E:148:ASP:H	1:H:18:GLN:HE22	1.61	0.49
1:E:10:VAL:HG22	1:E:88:VAL:HG21	1.93	0.49
1:F:95:THR:HA	1:F:106:ARG:NH1	2.28	0.49
1:G:47:GLU:O	1:G:51:GLU:HG3	2.13	0.49
1:H:48:LEU:HD12	1:H:48:LEU:O	2.12	0.49
1:H:54:ALA:O	1:H:55:GLU:C	2.50	0.49
1:C:65:LEU:HD11	3:C:1300:CDP:H1'	1.96	0.48
1:H:9:PHE:HZ	1:H:11:MET:HE2	1.77	0.48
1:G:53:TYR:OH	1:G:69:ILE:HD13	2.13	0.48
1:G:10:VAL:O	1:G:77:MET:N	2.46	0.48
1:F:18:GLN:NE2	1:G:147[A]:ARG:HG2	2.29	0.48
1:I:57:GLU:O	1:I:58:ASP:CB	2.62	0.47
1:B:78:VAL:HG21	1:B:142:LEU:HD21	1.95	0.47
1:C:5:ASP:O	1:C:7:ARG:HG3	2.14	0.47
1:C:109:TYR:HB3	1:C:117:LEU:HD21	1.96	0.47
1:G:11:MET:CE	1:G:69:ILE:HD11	2.43	0.47
1:F:69:ILE:HG23	1:F:69:ILE:O	2.13	0.47
1:F:17:VAL:HG21	1:F:73:PRO:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:GLN:HE22	1:G:147[A]:ARG:HG2	1.80	0.47
1:H:40:LYS:HG2	1:H:42:MET:CE	2.44	0.47
1:I:66:VAL:O	1:I:70:THR:HB	2.14	0.47
1:G:40:LYS:NZ	1:G:141:GLU:CD	2.68	0.47
1:C:106:ARG:HD3	1:C:116:ASN:HB2	1.96	0.47
1:H:7:ARG:HH21	1:H:142:LEU:HD13	1.80	0.47
1:D:11:MET:CE	1:D:69:ILE:HD11	2.45	0.46
1:A:81:GLY:O	1:A:84:ALA:HB2	2.15	0.46
1:C:35:LYS:NZ	1:C:80:GLU:OE2	2.46	0.46
1:F:8:THR:OG1	1:F:121:SER:HB2	2.16	0.46
1:H:67:SER:C	1:H:70:THR:HG22	2.36	0.46
1:G:152:TRP:NE1	1:I:18:GLN:HG2	2.31	0.46
1:B:7:ARG:HA	1:B:79:TRP:O	2.16	0.46
1:B:46:GLU:O	1:B:50:HIS:CD2	2.69	0.46
1:D:67:SER:O	1:D:70:THR:HG22	2.16	0.46
1:G:104:THR:HG22	1:I:102:PRO:HG3	1.98	0.46
1:A:11:MET:O	1:A:118:ILE:HA	2.16	0.46
1:F:117:LEU:C	1:F:118:ILE:HG22	2.35	0.46
1:G:6:GLU:HG2	1:G:84:ALA:HB3	1.98	0.46
1:C:40:LYS:HG2	4:C:1310:HOH:O	2.16	0.45
1:H:113:LEU:C	1:H:113:LEU:HD12	2.37	0.45
1:I:83:ASP:O	1:I:84:ALA:C	2.54	0.45
1:F:35:LYS:HG3	1:F:145:TRP:CZ2	2.51	0.45
1:F:4:HIS:HB2	1:F:80:GLU:OE2	2.15	0.45
1:A:40:LYS:NZ	1:A:141:GLU:OE2	2.50	0.45
1:F:29:LEU:HD21	1:F:88:VAL:HG22	1.99	0.45
1:F:7:ARG:NH1	1:F:142:LEU:HD13	2.32	0.45
1:F:14:PRO:HA	1:F:17:VAL:HG22	1.99	0.45
1:F:30:GLU:OE2	1:G:22:ILE:HG23	2.17	0.45
1:I:56:HIS:HA	1:I:59:LYS:HD2	1.98	0.45
1:A:18:GLN:HG3	1:B:152:TRP:CE2	2.51	0.45
1:G:32:LYS:NZ	1:G:87:GLN:OE1	2.49	0.44
1:E:44:ILE:HD13	1:E:69:ILE:HD13	1.99	0.44
1:E:92:MET:O	1:E:106:ARG:HB2	2.17	0.44
1:G:152:TRP:CD1	1:I:18:GLN:HG2	2.52	0.44
1:A:89:ARG:HD2	1:A:92:MET:CE	2.47	0.44
1:D:95:THR:HG21	3:D:1400:CDP:O3A	2.18	0.44
1:A:13:LYS:HB3	1:A:14:PRO:CD	2.48	0.43
1:A:147:ARG:O	1:A:150:SER:HB2	2.17	0.43
1:B:27:THR:O	1:B:31:THR:HB	2.17	0.43
1:E:78:VAL:HG21	1:E:142:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:ALA:O	1:E:88:VAL:HG13	2.18	0.43
1:I:13:LYS:HB3	1:I:14:PRO:HD2	2.00	0.43
1:G:32:LYS:CE	1:I:110:GLY:O	2.66	0.43
1:D:29:LEU:HD22	1:D:34:LEU:HD12	2.00	0.43
1:G:32:LYS:HE2	1:I:110:GLY:O	2.19	0.43
1:C:35:LYS:HG3	1:C:145:TRP:CZ2	2.54	0.43
1:I:10:VAL:HG22	1:I:88:VAL:HG11	2.00	0.43
1:C:6:GLU:O	1:C:80:GLU:HA	2.19	0.43
1:F:40:LYS:HB3	1:F:42:MET:HE2	1.99	0.43
1:A:10:VAL:HG22	1:A:77:MET:HE3	2.00	0.43
1:B:17:VAL:HG13	1:B:22:ILE:HD11	2.00	0.43
1:F:32:LYS:HD3	1:F:91:LEU:HD21	2.01	0.43
1:E:109:TYR:HD1	1:F:31:THR:HG22	1.84	0.43
1:I:78:VAL:HG23	1:I:137:PHE:CE2	2.54	0.43
1:B:18:GLN:HG2	4:B:1206:HOH:O	2.18	0.43
1:B:6:GLU:O	1:B:80:GLU:HA	2.19	0.43
1:E:6:GLU:O	1:E:80:GLU:HA	2.19	0.43
1:F:117:LEU:HB3	1:F:118:ILE:HG22	2.00	0.42
1:G:7:ARG:NH1	1:G:142:LEU:HD13	2.33	0.42
1:I:48:LEU:CD1	1:I:135:LEU:CD2	2.97	0.42
1:I:135:LEU:O	1:I:135:LEU:CD2	2.59	0.42
1:I:29:LEU:CD2	1:I:88:VAL:HG22	2.49	0.42
1:D:128:ALA:O	1:D:132:GLU:HG3	2.19	0.42
1:A:40:LYS:HZ1	1:A:141:GLU:CD	2.22	0.42
1:G:78:VAL:HG22	1:G:133:ILE:HG12	2.01	0.42
1:A:10:VAL:HG13	1:A:79:TRP:CD1	2.49	0.42
1:D:91:LEU:HD13	4:D:1410:HOH:O	2.20	0.42
1:F:13:LYS:HD3	1:F:68:PHE:HE2	1.84	0.42
1:F:145:TRP:CH2	1:F:147:ARG:HG2	2.55	0.42
1:H:17:VAL:HG22	1:H:22:ILE:HD11	2.01	0.42
1:H:54:ALA:C	1:H:56:HIS:N	2.73	0.42
1:H:9:PHE:HZ	1:H:11:MET:CE	2.32	0.42
1:C:13:LYS:HE3	1:C:118:ILE:O	2.20	0.41
1:C:22:ILE:O	1:C:26:VAL:HG23	2.19	0.41
1:F:83:ASP:OD2	1:F:86:ARG:NE	2.41	0.41
1:G:44:ILE:HD12	1:G:74:VAL:HG11	2.02	0.41
1:H:89:ARG:NH2	1:H:122:ASP:HB2	2.34	0.41
1:A:128:ALA:O	1:A:132:GLU:CG	2.59	0.41
1:A:32:LYS:HG3	1:A:32:LYS:O	2.19	0.41
1:D:68:PHE:O	1:D:71:SER:OG	2.29	0.41
1:H:83:ASP:OD2	1:H:86[B]:ARG:NE	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:TYR:CZ	1:C:65:LEU:HD21	2.54	0.41
1:D:40:LYS:HZ3	1:D:40:LYS:HB2	1.86	0.41
1:I:86:ARG:HH11	1:I:90:GLN:HE22	1.67	0.41
1:D:147:ARG:HA	1:I:18:GLN:NE2	2.35	0.41
1:F:13:LYS:HZ1	1:F:119:HIS:HB2	1.85	0.41
1:H:54:ALA:O	1:H:56:HIS:N	2.54	0.41
1:I:44:ILE:HD12	1:I:74:VAL:HG21	2.02	0.41
1:H:105:ILE:HD13	1:H:118:ILE:HD13	2.02	0.41
1:I:48:LEU:CD1	1:I:135:LEU:HD22	2.51	0.41
1:F:10:VAL:HG22	1:F:88:VAL:HG11	2.03	0.41
1:A:89:ARG:HD2	1:A:92:MET:HE1	2.03	0.41
1:E:65:LEU:HD13	3:E:1500:CDP:H1'	2.02	0.41
1:F:116:ASN:O	1:F:117:LEU:HB2	2.21	0.41
1:A:10:VAL:HG22	1:A:77:MET:CE	2.51	0.41
1:H:27:THR:O	1:H:31:THR:HB	2.21	0.41
1:I:65:LEU:HD23	1:I:65:LEU:C	2.40	0.41
1:F:118:ILE:HD13	1:F:118:ILE:HG21	1.79	0.40
1:I:113:LEU:CD2	1:I:113:LEU:O	2.69	0.40
1:C:50:HIS:CE1	4:C:1304:HOH:O	2.73	0.40
1:D:13:LYS:O	1:D:14:PRO:C	2.60	0.40
1:B:78:VAL:HG21	1:B:142:LEU:CD2	2.51	0.40
1:F:7:ARG:O	1:F:129:ASN:HB2	2.21	0.40
1:H:101:ALA:O	1:H:104:THR:HG23	2.22	0.40
1:A:149:ALA:O	1:A:153:VAL:HG23	2.21	0.40
1:H:86[B]:ARG:NH1	1:H:90:GLN:NE2	2.68	0.40
1:C:111:ASN:OD1	1:C:111:ASN:N	2.54	0.40
1:F:91:LEU:O	1:F:105:ILE:HG12	2.22	0.40
1:G:106:ARG:NH2	1:G:118:ILE:O	2.51	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	150/164 (92%)	143 (95%)	6 (4%)	1 (1%)	22	22
1	B	149/164 (91%)	144 (97%)	5 (3%)	0	100	100
1	C	151/164 (92%)	146 (97%)	5 (3%)	0	100	100
1	D	150/164 (92%)	143 (95%)	7 (5%)	0	100	100
1	E	150/164 (92%)	147 (98%)	2 (1%)	1 (1%)	22	22
1	F	150/164 (92%)	144 (96%)	5 (3%)	1 (1%)	22	22
1	G	151/164 (92%)	147 (97%)	4 (3%)	0	100	100
1	H	151/164 (92%)	144 (95%)	5 (3%)	2 (1%)	12	9
1	I	149/164 (91%)	142 (95%)	6 (4%)	1 (1%)	22	22
All	All	1351/1476 (92%)	1300 (96%)	45 (3%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	55	GLU
1	E	117	LEU
1	I	58	ASP
1	A	150	SER
1	H	60	PRO
1	F	117	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/133 (90%)	113 (94%)	7 (6%)	20	23
1	B	122/133 (92%)	112 (92%)	10 (8%)	11	11
1	C	123/133 (92%)	111 (90%)	12 (10%)	8	7
1	D	121/133 (91%)	111 (92%)	10 (8%)	11	11
1	E	120/133 (90%)	110 (92%)	10 (8%)	11	11
1	F	123/133 (92%)	108 (88%)	15 (12%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	122/133 (92%)	112 (92%)	10 (8%)	11	11
1	H	120/133 (90%)	110 (92%)	10 (8%)	11	11
1	I	120/133 (90%)	110 (92%)	10 (8%)	11	11
All	All	1091/1197 (91%)	997 (91%)	94 (9%)	10	10

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	31	THR
1	A	115	HIS
1	A	118	ILE
1	A	140	ASP
1	A	141	GLU
1	A	144	ASP
1	B	7	ARG
1	B	11	MET
1	B	48	LEU
1	B	51	GLU
1	B	57	GLU
1	B	59	LYS
1	B	70	THR
1	B	80	GLU
1	B	117	LEU
1	B	124	GLU
1	C	7	ARG
1	C	18	GLN
1	C	31	THR
1	C	40	LYS
1	C	65	LEU
1	C	70	THR
1	C	89	ARG
1	C	91	LEU
1	C	126	GLU
1	C	140	ASP
1	C	144	ASP
1	C	147	ARG
1	D	7	ARG
1	D	27	THR
1	D	45	ASP
1	D	69	ILE

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Mol	Chain	Res	Type
1	D	74	VAL
1	D	91	LEU
1	D	95	THR
1	D	135	LEU
1	D	140	ASP
1	D	147	ARG
1	E	5	ASP
1	E	11	MET
1	E	18	GLN
1	E	69	ILE
1	E	70	THR
1	E	95	THR
1	E	113	LEU
1	E	138	ASP
1	E	139	ASP
1	E	147	ARG
1	F	5	ASP
1	F	11	MET
1	F	37	VAL
1	F	46	GLU
1	F	63	ASP
1	F	86	ARG
1	F	95	THR
1	F	115	HIS
1	F	117	LEU
1	F	118	ILE
1	F	126	GLU
1	F	135	LEU
1	F	140	ASP
1	F	146	ASP
1	F	147	ARG
1	G	4	HIS
1	G	22	ILE
1	G	40	LYS
1	G	43	ARG
1	G	47	GLU
1	G	69	ILE
1	G	113	LEU
1	G	115	HIS
1	G	146	ASP
1	G	155	GLU
1	H	5	ASP

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Mol	Chain	Res	Type
1	H	7	ARG
1	H	18	GLN
1	H	31	THR
1	H	40	LYS
1	H	42	MET
1	H	43	ARG
1	H	48	LEU
1	H	67	SER
1	H	89	ARG
1	I	28	ARG
1	I	43	ARG
1	I	51	GLU
1	I	56	HIS
1	I	74	VAL
1	I	89	ARG
1	I	95	THR
1	I	113	LEU
1	I	115	HIS
1	I	148	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	B	18	GLN
1	B	50	HIS
1	B	52	HIS
1	B	123	HIS
1	C	18	GLN
1	D	50	HIS
1	F	18	GLN
1	F	50	HIS
1	G	18	GLN
1	G	50	HIS
1	G	115	HIS
1	H	18	GLN
1	H	50	HIS
1	H	90	GLN
1	I	18	GLN
1	I	90	GLN
1	I	115	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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$
3	CDP	B	1200	2	21,26,26	1.25	2 (9%)	28,40,40	1.83	6 (21%)
3	CDP	A	1100	2	21,26,26	1.46	3 (14%)	28,40,40	1.48	2 (7%)
3	CDP	H	1800	-	21,26,26	1.30	3 (14%)	28,40,40	1.45	3 (10%)
3	CDP	I	1900	-	21,26,26	1.21	2 (9%)	28,40,40	1.57	3 (10%)
3	CDP	C	1300	-	21,26,26	1.33	3 (14%)	28,40,40	1.76	5 (17%)
3	CDP	E	1500	-	21,26,26	1.26	2 (9%)	28,40,40	1.89	7 (25%)
3	CDP	F	1600	-	21,26,26	1.25	2 (9%)	28,40,40	1.95	5 (17%)
3	CDP	G	1700	-	21,26,26	1.37	3 (14%)	28,40,40	1.55	6 (21%)
3	CDP	D	1400	-	21,26,26	1.26	2 (9%)	28,40,40	1.96	4 (14%)

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	CDP	B	1200	2	-	0/14/32/32	0/2/2/2
3	CDP	A	1100	2	-	3/14/32/32	0/2/2/2
3	CDP	H	1800	-	-	3/14/32/32	0/2/2/2
3	CDP	I	1900	-	-	8/14/32/32	0/2/2/2
3	CDP	C	1300	-	-	3/14/32/32	0/2/2/2
3	CDP	E	1500	-	-	3/14/32/32	0/2/2/2
3	CDP	F	1600	-	-	6/14/32/32	0/2/2/2
3	CDP	G	1700	-	-	5/14/32/32	0/2/2/2
3	CDP	D	1400	-	-	5/14/32/32	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1500	CDP	PB-O1B	3.68	1.62	1.50
3	D	1400	CDP	PB-O1B	3.48	1.61	1.50
3	G	1700	CDP	O4'-C1'	3.39	1.45	1.41
3	F	1600	CDP	PB-O1B	3.29	1.61	1.50
3	A	1100	CDP	PB-O1B	3.22	1.60	1.50
3	G	1700	CDP	PA-O1A	2.97	1.61	1.50
3	A	1100	CDP	PA-O1A	2.96	1.61	1.50
3	C	1300	CDP	PB-O1B	2.95	1.60	1.50
3	H	1800	CDP	PB-O1B	2.93	1.60	1.50
3	I	1900	CDP	PB-O1B	2.89	1.59	1.50
3	F	1600	CDP	PA-O1A	2.82	1.60	1.50
3	D	1400	CDP	PA-O1A	2.78	1.60	1.50
3	I	1900	CDP	PA-O1A	2.72	1.60	1.50
3	G	1700	CDP	PB-O1B	2.70	1.59	1.50
3	B	1200	CDP	PB-O1B	2.66	1.59	1.50
3	C	1300	CDP	PA-O1A	2.61	1.60	1.50
3	E	1500	CDP	PA-O1A	2.61	1.60	1.50
3	H	1800	CDP	PA-O1A	2.57	1.60	1.50
3	C	1300	CDP	C6-N1	-2.52	1.32	1.35
3	H	1800	CDP	O4'-C1'	2.26	1.44	1.41
3	B	1200	CDP	O4'-C1'	2.25	1.44	1.41
3	A	1100	CDP	C2-N3	-2.09	1.34	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1400	CDP	C2-N3-C4	6.75	123.18	116.34
3	F	1600	CDP	C2-N3-C4	6.42	122.84	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1200	CDP	C3'-C2'-C1'	5.83	109.75	100.98
3	C	1300	CDP	C3'-C2'-C1'	5.40	109.11	100.98
3	E	1500	CDP	C2-N3-C4	4.88	121.29	116.34
3	A	1100	CDP	C3'-C2'-C1'	4.83	108.25	100.98
3	I	1900	CDP	C3'-C2'-C1'	4.61	107.92	100.98
3	D	1400	CDP	C3'-C2'-C1'	4.43	107.64	100.98
3	G	1700	CDP	C3'-C2'-C1'	4.29	107.44	100.98
3	I	1900	CDP	C2-N3-C4	4.27	120.67	116.34
3	C	1300	CDP	C2-N3-C4	4.18	120.57	116.34
3	H	1800	CDP	C3'-C2'-C1'	3.95	106.93	100.98
3	E	1500	CDP	C3'-C2'-C1'	3.93	106.89	100.98
3	E	1500	CDP	PA-O3A-PB	-3.90	119.46	132.83
3	F	1600	CDP	C3'-C2'-C1'	3.67	106.50	100.98
3	B	1200	CDP	C2-N3-C4	3.61	120.00	116.34
3	D	1400	CDP	PA-O3A-PB	-3.40	121.17	132.83
3	D	1400	CDP	C5-C4-N3	-3.30	117.91	121.72
3	G	1700	CDP	C2-N3-C4	3.21	119.60	116.34
3	H	1800	CDP	C2-N3-C4	3.15	119.54	116.34
3	G	1700	CDP	O3B-PB-O3A	3.04	114.82	104.64
3	F	1600	CDP	O3'-C3'-C4'	3.00	119.72	111.05
3	G	1700	CDP	PA-O3A-PB	-2.89	122.91	132.83
3	C	1300	CDP	O2'-C2'-C3'	-2.88	102.52	111.82
3	H	1800	CDP	O3B-PB-O3A	2.85	114.21	104.64
3	E	1500	CDP	O4'-C4'-C3'	2.69	110.44	105.11
3	I	1900	CDP	O3B-PB-O3A	2.53	113.13	104.64
3	B	1200	CDP	O2B-PB-O3B	2.51	117.22	107.64
3	C	1300	CDP	PA-O3A-PB	-2.50	124.23	132.83
3	B	1200	CDP	O4'-C4'-C5'	2.49	117.57	109.37
3	E	1500	CDP	O5'-C5'-C4'	2.48	117.53	108.99
3	F	1600	CDP	C5-C4-N3	-2.33	119.03	121.72
3	C	1300	CDP	O3'-C3'-C4'	2.31	117.74	111.05
3	F	1600	CDP	O4'-C4'-C3'	2.31	109.68	105.11
3	E	1500	CDP	PA-O5'-C5'	-2.24	108.57	121.68
3	G	1700	CDP	C6-N1-C2	-2.15	117.78	121.20
3	A	1100	CDP	C5-C4-N4	2.14	124.85	121.14
3	B	1200	CDP	O2'-C2'-C1'	-2.14	102.96	110.85
3	B	1200	CDP	O2'-C2'-C3'	-2.08	105.09	111.82
3	E	1500	CDP	O2A-PA-O5'	2.07	117.35	107.75
3	G	1700	CDP	C2'-C3'-C4'	2.01	106.54	102.64

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1100	CDP	O4'-C1'-N1-C6
3	I	1900	CDP	PA-O3A-PB-O2B
3	I	1900	CDP	C5'-O5'-PA-O1A
3	I	1900	CDP	C2'-C1'-N1-C6
3	H	1800	CDP	O4'-C1'-N1-C6
3	E	1500	CDP	C5'-O5'-PA-O1A
3	F	1600	CDP	C5'-O5'-PA-O1A
3	F	1600	CDP	C5'-O5'-PA-O2A
3	F	1600	CDP	O4'-C4'-C5'-O5'
3	D	1400	CDP	C5'-O5'-PA-O1A
3	G	1700	CDP	C5'-O5'-PA-O1A
3	G	1700	CDP	O4'-C1'-N1-C6
3	I	1900	CDP	O4'-C4'-C5'-O5'
3	F	1600	CDP	C3'-C4'-C5'-O5'
3	I	1900	CDP	C4'-C5'-O5'-PA
3	D	1400	CDP	O4'-C4'-C5'-O5'
3	I	1900	CDP	C3'-C4'-C5'-O5'
3	C	1300	CDP	PA-O3A-PB-O1B
3	I	1900	CDP	C5'-O5'-PA-O3A
3	E	1500	CDP	C5'-O5'-PA-O3A
3	G	1700	CDP	C5'-O5'-PA-O3A
3	A	1100	CDP	PB-O3A-PA-O1A
3	F	1600	CDP	PB-O3A-PA-O1A
3	I	1900	CDP	C5'-O5'-PA-O2A
3	E	1500	CDP	C5'-O5'-PA-O2A
3	D	1400	CDP	C5'-O5'-PA-O2A
3	G	1700	CDP	C5'-O5'-PA-O2A
3	D	1400	CDP	C3'-C4'-C5'-O5'
3	A	1100	CDP	PA-O3A-PB-O2B
3	C	1300	CDP	PA-O3A-PB-O3B
3	C	1300	CDP	PA-O3A-PB-O2B
3	F	1600	CDP	C5'-O5'-PA-O3A
3	D	1400	CDP	C5'-O5'-PA-O3A
3	H	1800	CDP	C4'-C5'-O5'-PA
3	G	1700	CDP	PB-O3A-PA-O2A
3	H	1800	CDP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 8 short contacts:

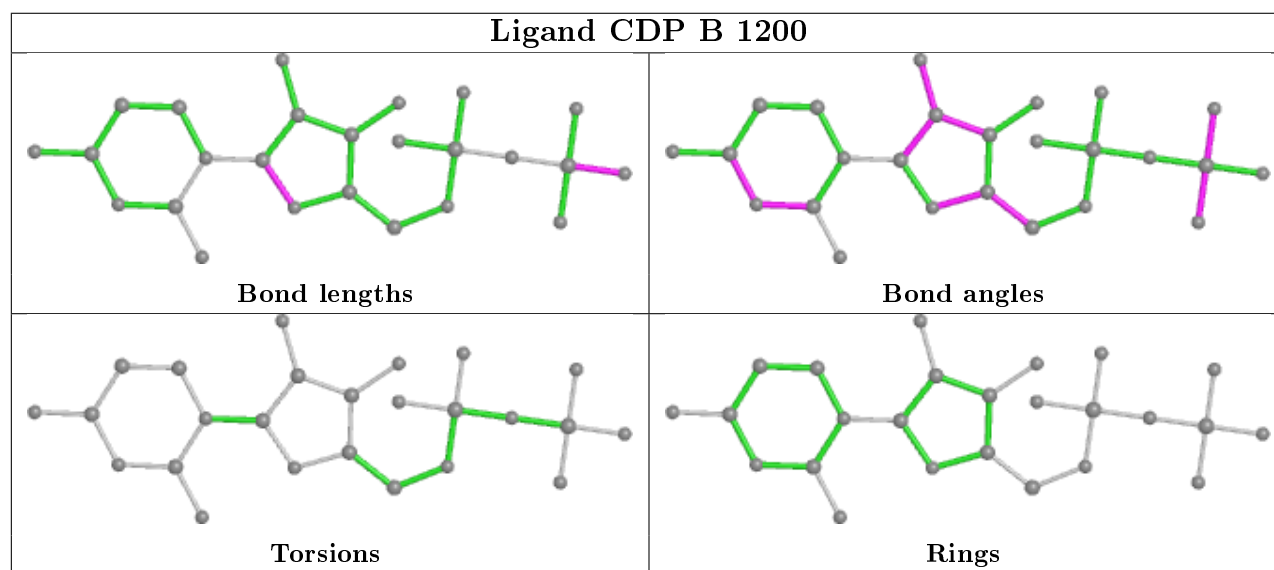
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1300	CDP	3	0
3	E	1500	CDP	2	0

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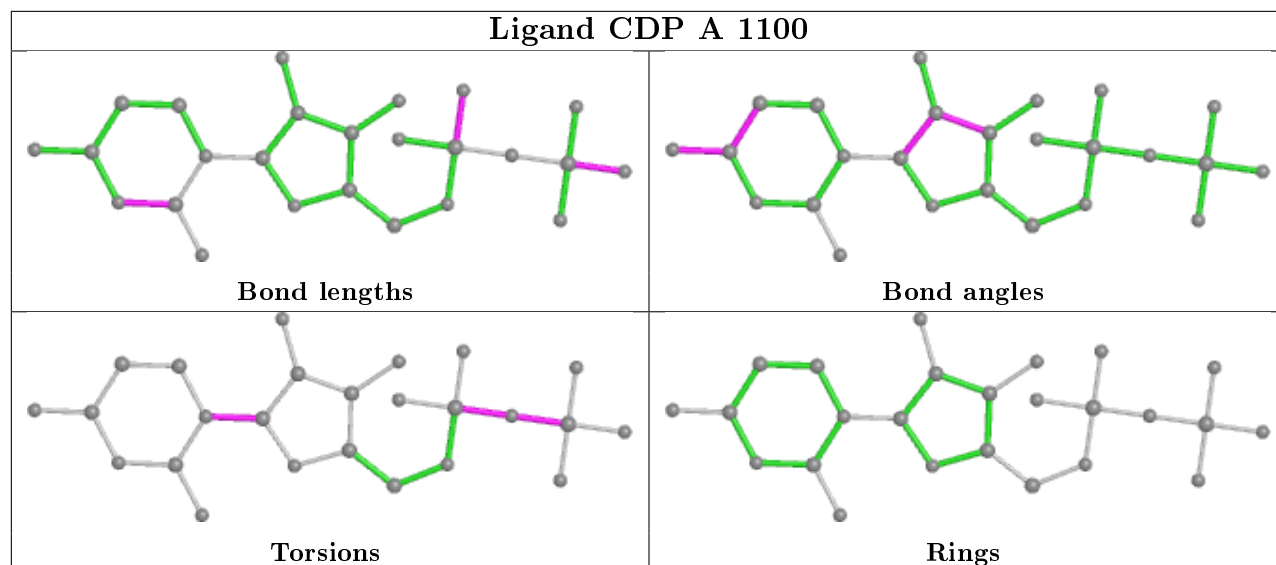
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1700	CDP	1	0
3	D	1400	CDP	2	0

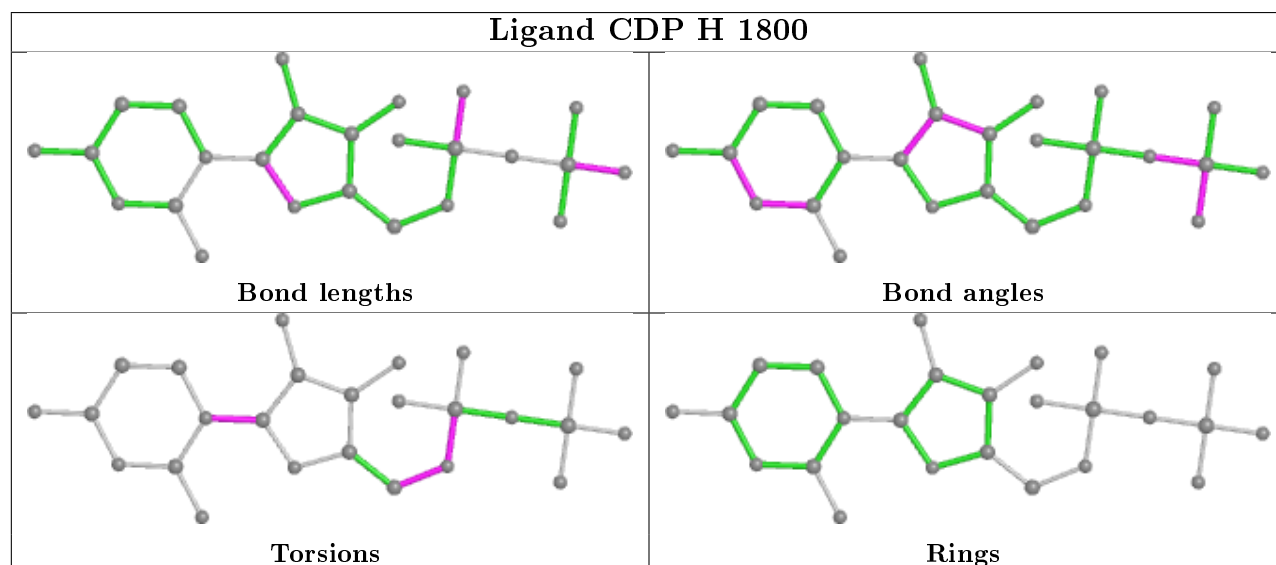
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



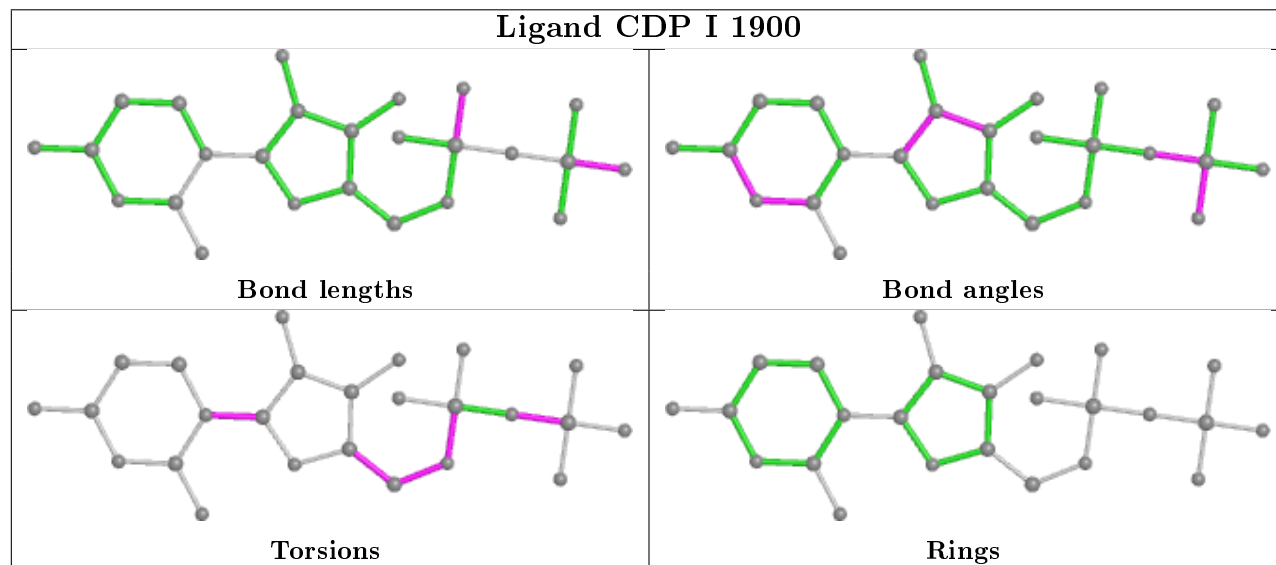
Ligand CDP A 1100



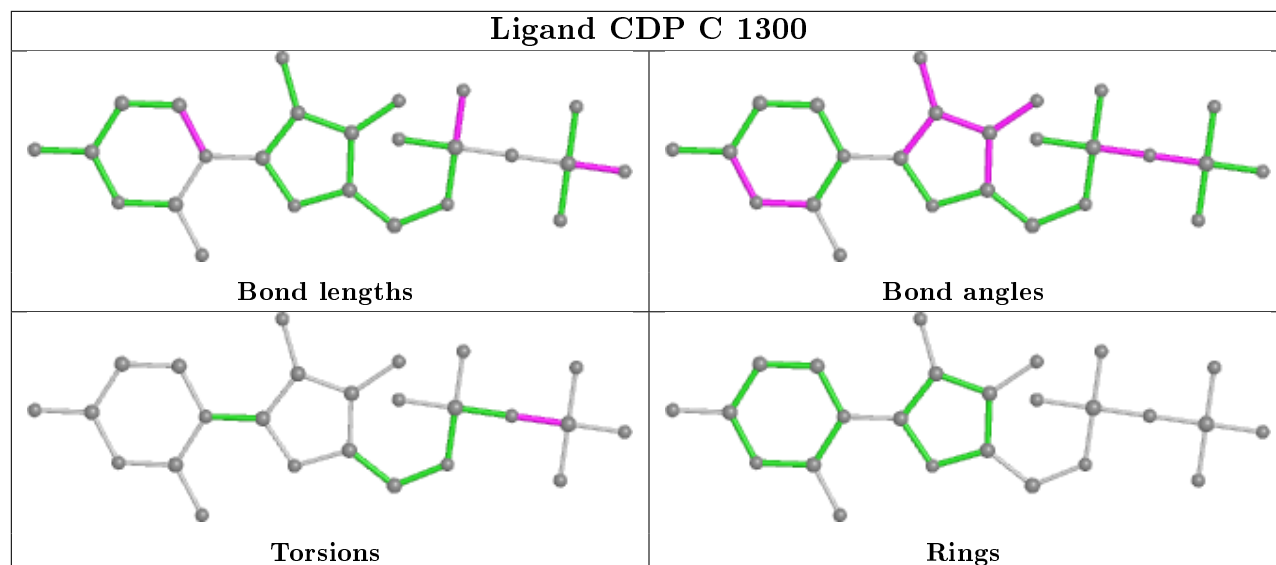
Ligand CDP H 1800



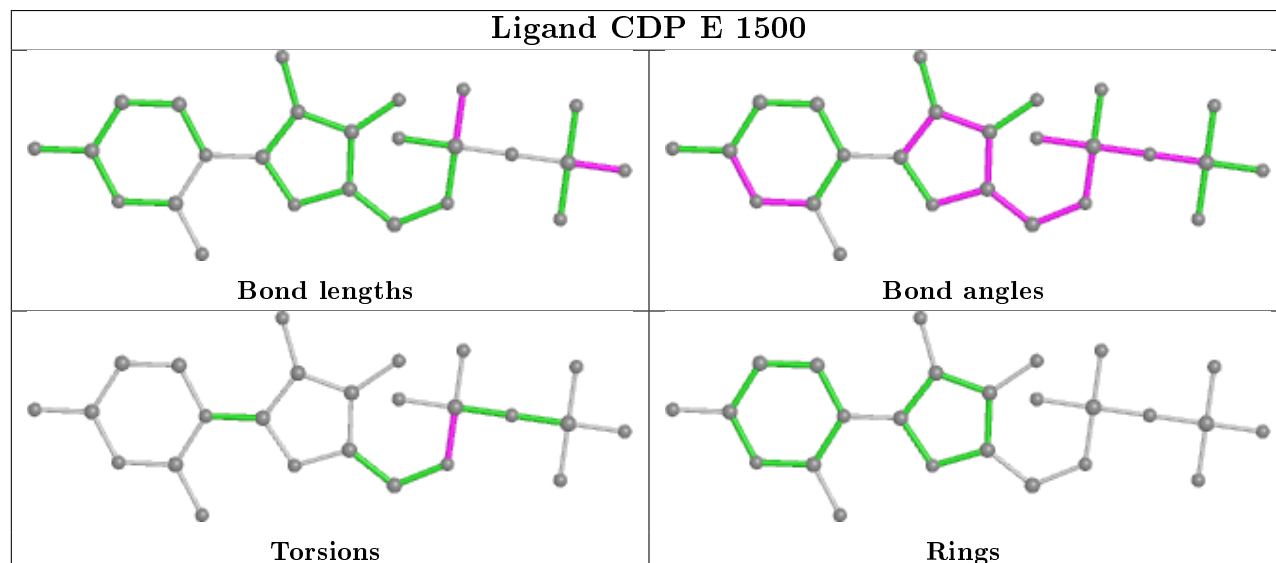
Ligand CDP I 1900



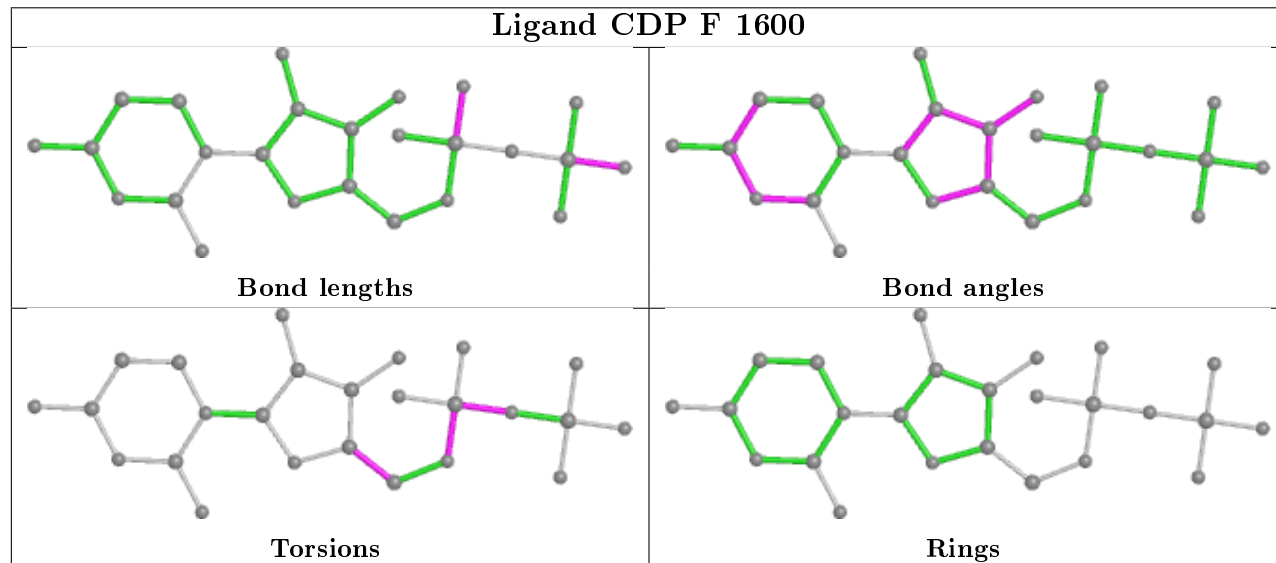
Ligand CDP C 1300

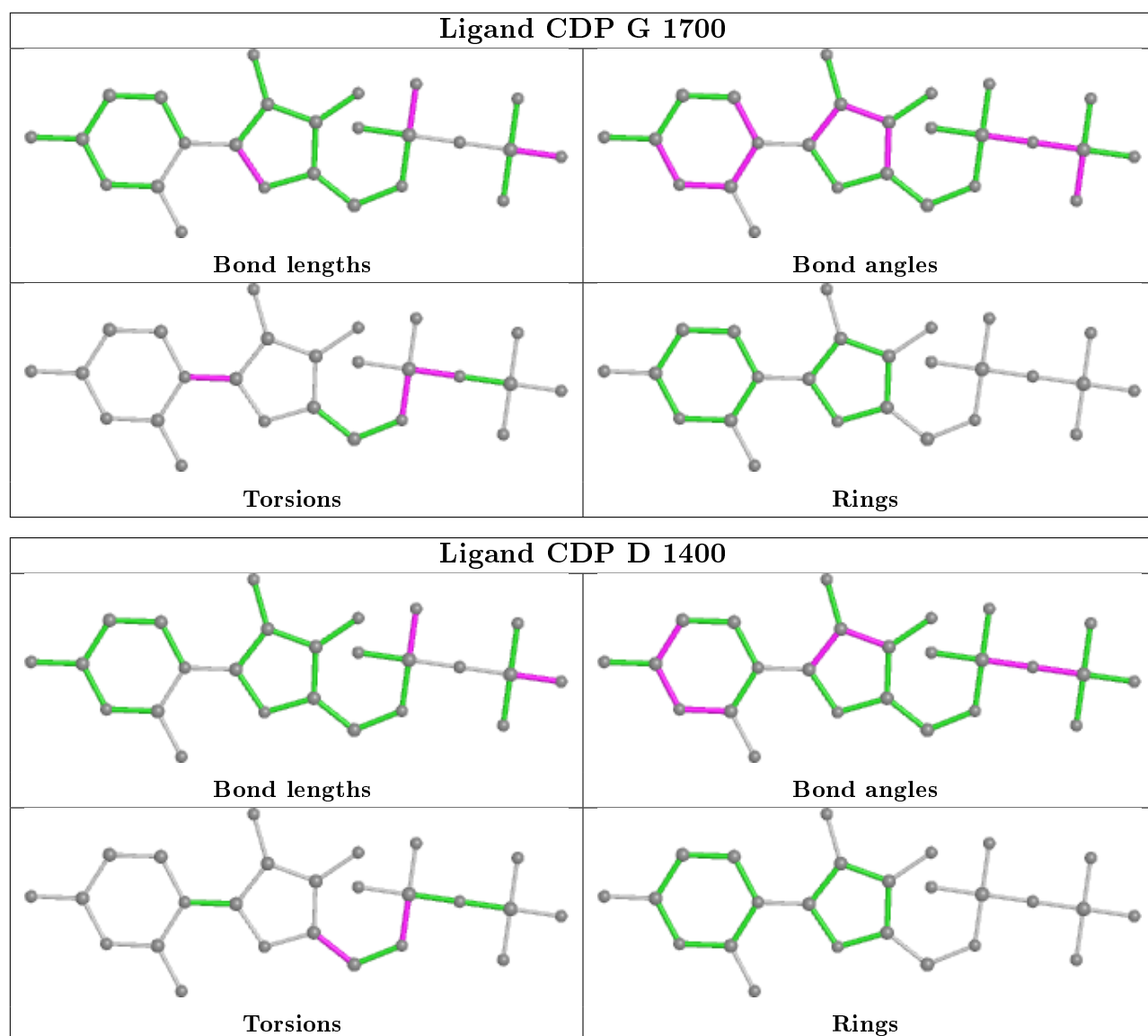


Ligand CDP E 1500



Ligand CDP F 1600





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	152/164 (92%)	-0.35	1 (0%) 87 86	23, 31, 48, 50	0
1	B	151/164 (92%)	-0.36	0 100 100	24, 32, 48, 55	0
1	C	153/164 (93%)	-0.31	0 100 100	24, 32, 49, 57	0
1	D	152/164 (92%)	-0.26	0 100 100	29, 39, 52, 55	0
1	E	152/164 (92%)	-0.23	0 100 100	29, 41, 52, 57	0
1	F	152/164 (92%)	-0.28	1 (0%) 87 86	28, 39, 52, 63	0
1	G	152/164 (92%)	-0.21	1 (0%) 87 86	31, 41, 59, 68	0
1	H	152/164 (92%)	-0.21	0 100 100	32, 41, 57, 62	0
1	I	151/164 (92%)	-0.24	0 100 100	32, 41, 57, 61	0
All	All	1367/1476 (92%)	-0.27	3 (0%) 95 94	23, 38, 54, 68	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	4	HIS	4.1
1	G	4	HIS	3.8
1	A	4	HIS	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](#)

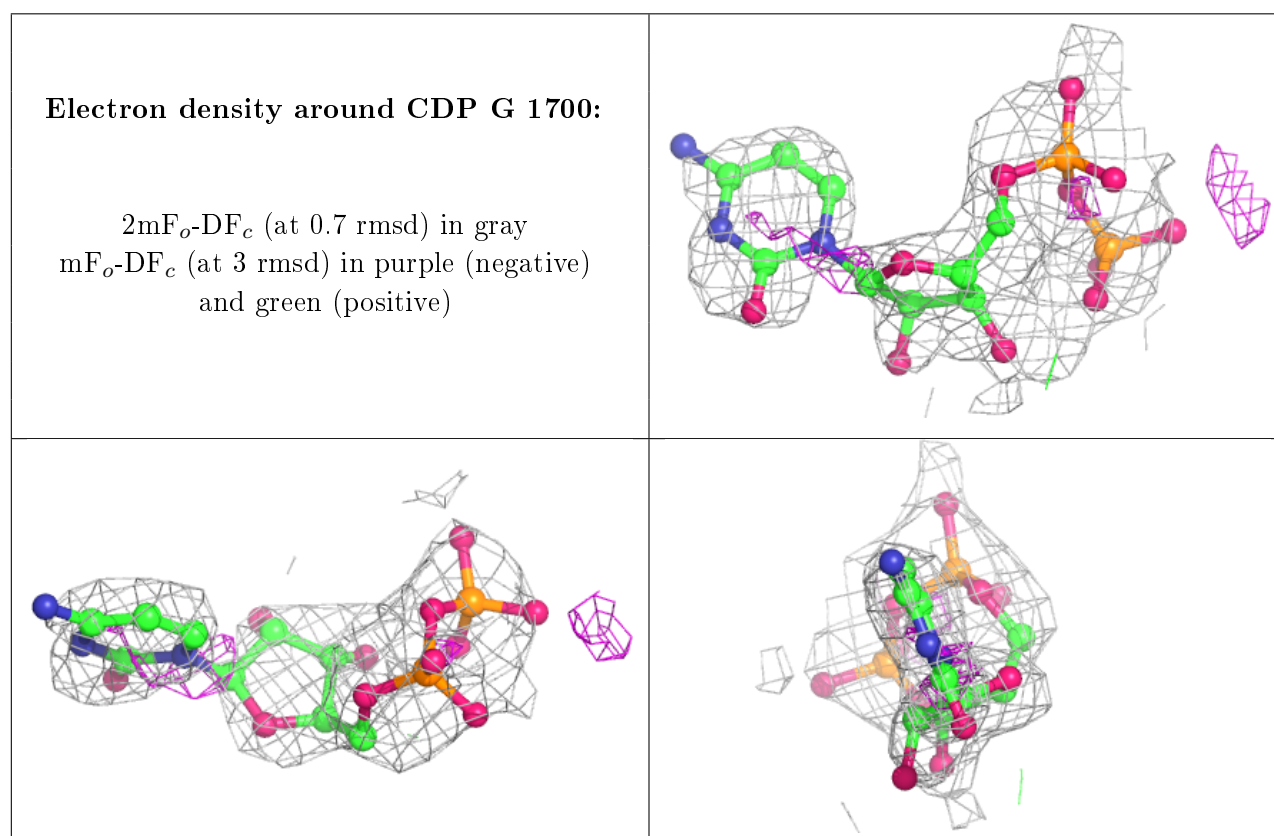
There are no carbohydrates in this entry.

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.

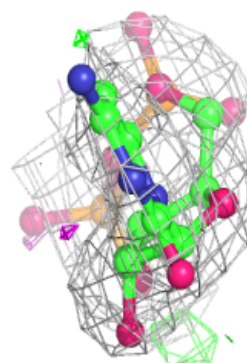
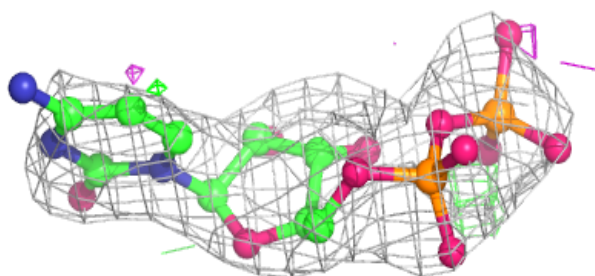
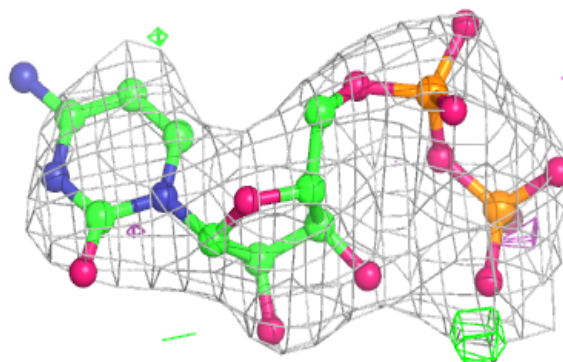
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CDP	G	1700	25/25	0.84	0.22	75,78,86,86	0
3	CDP	I	1900	25/25	0.88	0.19	81,82,88,89	0
3	CDP	H	1800	25/25	0.90	0.12	59,65,73,73	0
2	MG	B	202	1/1	0.91	0.09	42,42,42,42	0
3	CDP	D	1400	25/25	0.92	0.13	46,52,57,60	0
3	CDP	E	1500	25/25	0.93	0.10	43,53,55,57	0
3	CDP	F	1600	25/25	0.93	0.11	45,52,58,60	0
2	MG	A	201	1/1	0.94	0.14	43,43,43,43	0
3	CDP	A	1100	25/25	0.96	0.11	33,40,54,57	0
3	CDP	B	1200	25/25	0.97	0.11	29,37,48,52	0
3	CDP	C	1300	25/25	0.97	0.11	34,39,49,50	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.

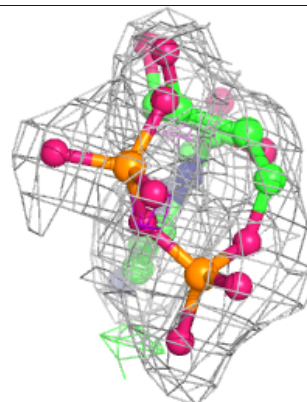
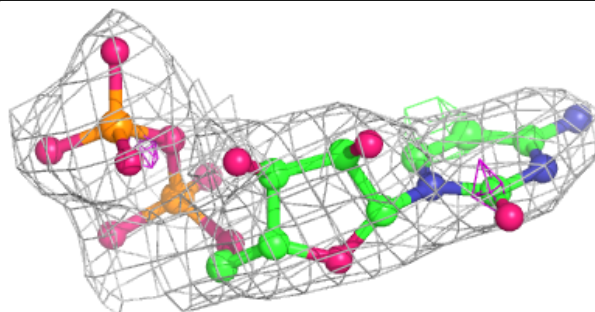
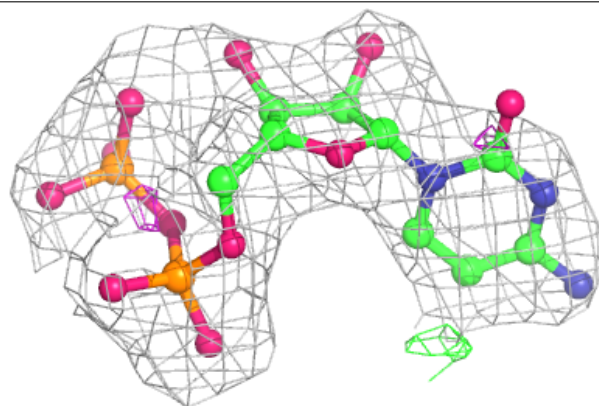


Electron density around CDP I 1900:

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

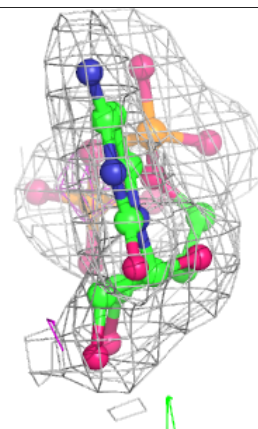
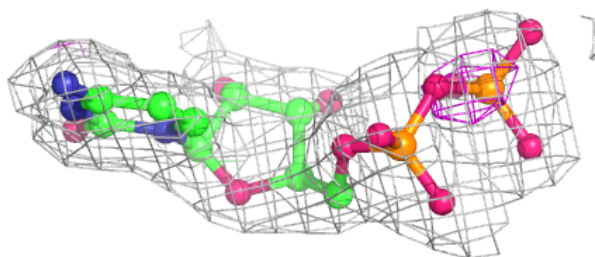
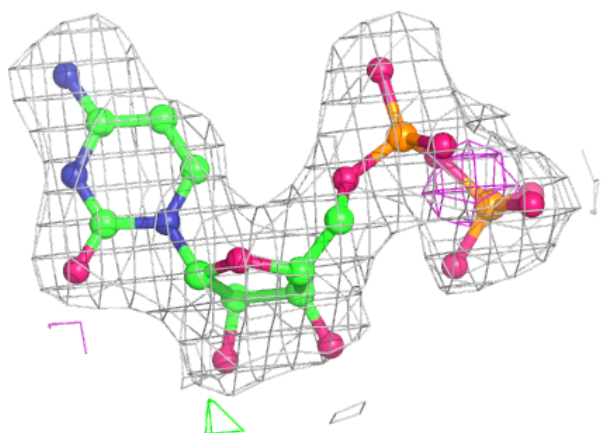
**Electron density around CDP H 1800:**

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



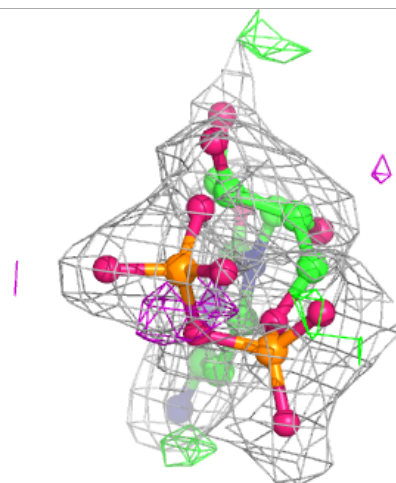
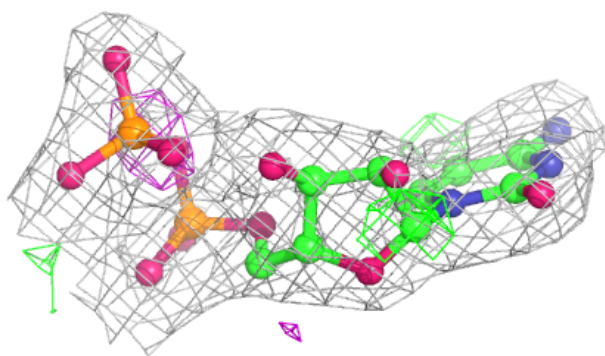
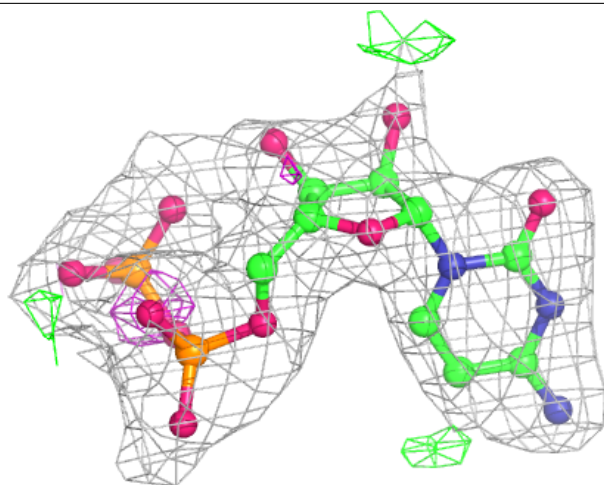
Electron density around CDP D 1400:

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



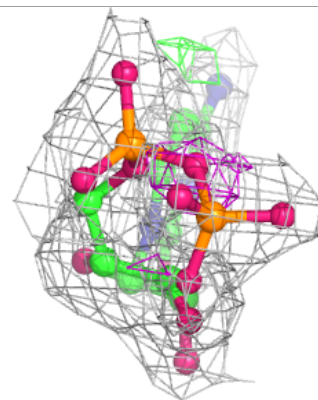
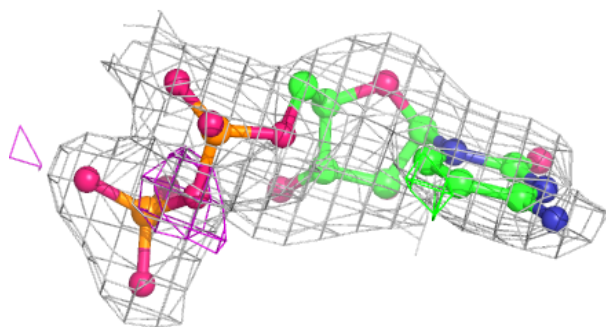
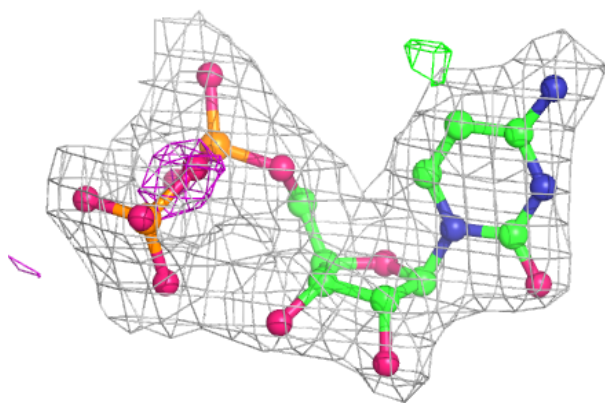
Electron density around CDP E 1500:

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

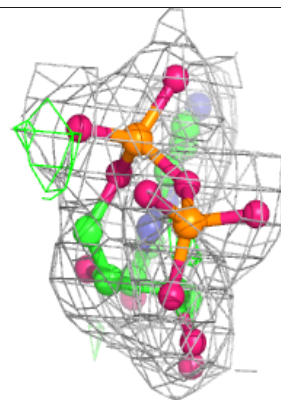
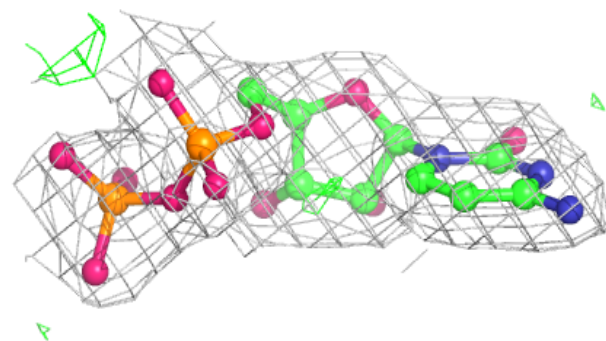
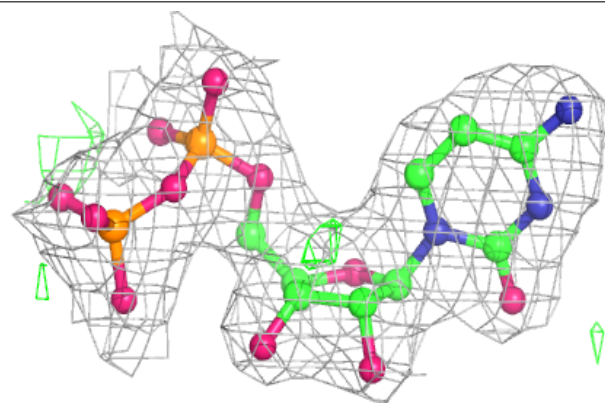


Electron density around CDP F 1600:

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

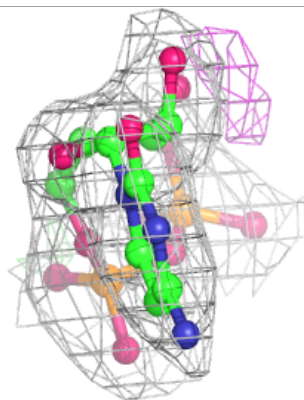
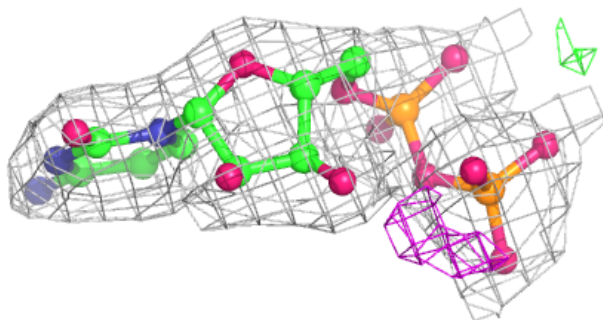
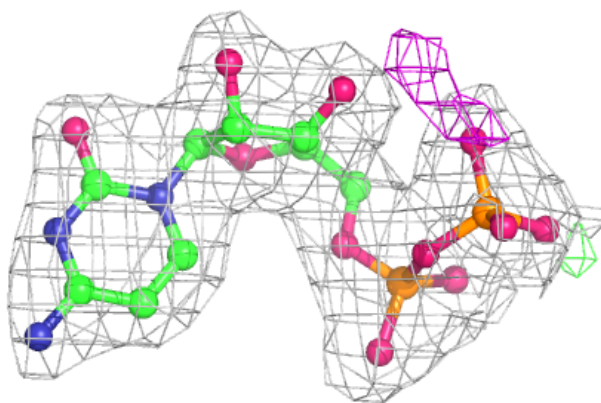
**Electron density around CDP A 1100:**

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

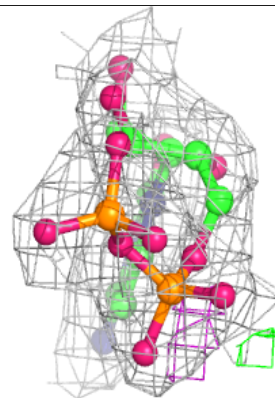
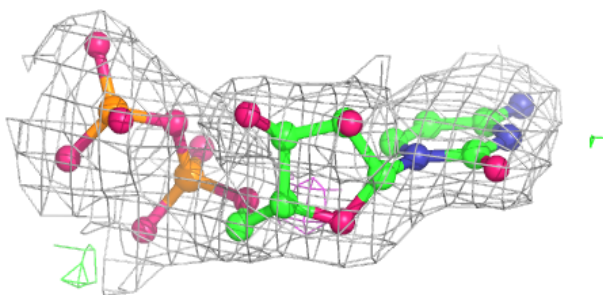
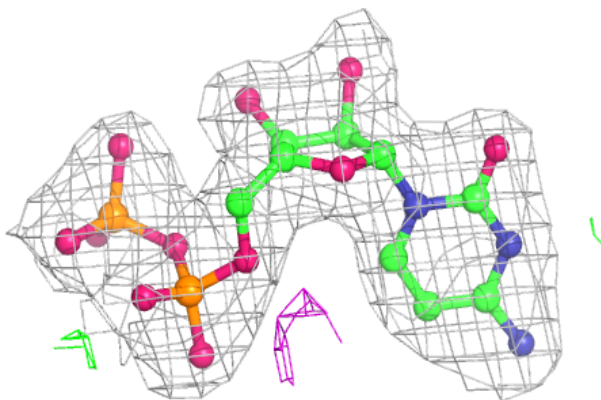


Electron density around CDP B 1200:

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

**Electron density around CDP C 1300:**

$2mF_o-DF_c$ (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.