



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:06 am BST

PDB ID : 5K8B
Title : X-ray structure of KdnA, 8-amino-3,8-dideoxy-alpha-D-manno-octulosonate transaminase, from *Shewanella oneidensis* in the presence of the external aldimine with PLP and glutamate
Authors : Holden, H.M.; Thoden, J.B.; Zachman-Brockmeyer, T.R.
Deposited on : 2016-05-28
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

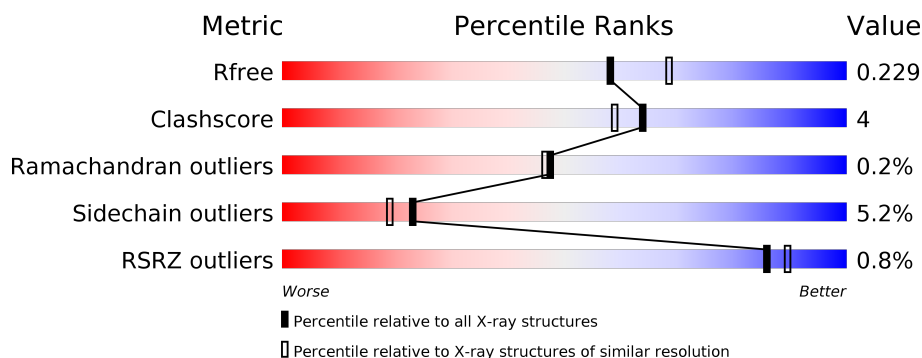
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	403	<div> <div>85%</div> <div>9%</div> <div>• •</div> </div>
1	B	403	<div> <div>83%</div> <div>14%</div> <div>• •</div> </div>
1	C	403	<div> <div>84%</div> <div>12%</div> <div>• • •</div> </div>
1	D	403	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>• •</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13031 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 8-amino-3,8-dideoxy-alpha-D-manno-octulosonate transaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	1	0
			3054	1933	521	575	25			
1	B	394	Total	C	N	O	S	0	1	0
			3053	1932	522	574	25			
1	C	394	Total	C	N	O	S	0	1	0
			3054	1933	521	575	25			
1	D	394	Total	C	N	O	S	0	1	0
			3054	1933	521	575	25			

There are 32 discrepancies between the modelled and reference sequences:

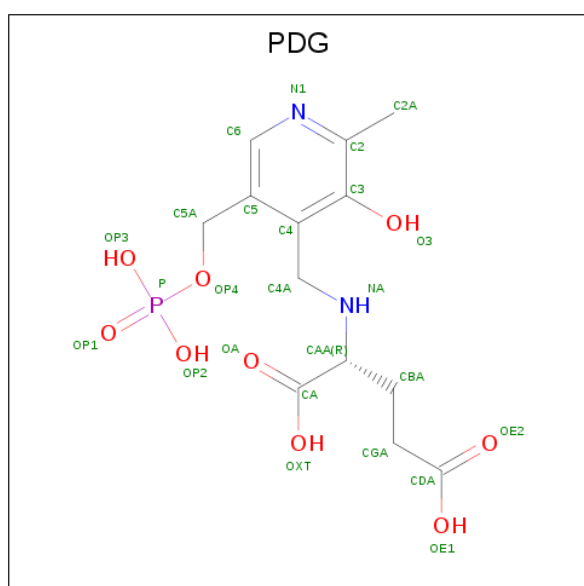
Chain	Residue	Modelled	Actual	Comment	Reference
A	396	LEU	-	expression tag	UNP Q8EEB1
A	397	GLU	-	expression tag	UNP Q8EEB1
A	398	HIS	-	expression tag	UNP Q8EEB1
A	399	HIS	-	expression tag	UNP Q8EEB1
A	400	HIS	-	expression tag	UNP Q8EEB1
A	401	HIS	-	expression tag	UNP Q8EEB1
A	402	HIS	-	expression tag	UNP Q8EEB1
A	403	HIS	-	expression tag	UNP Q8EEB1
B	396	LEU	-	expression tag	UNP Q8EEB1
B	397	GLU	-	expression tag	UNP Q8EEB1
B	398	HIS	-	expression tag	UNP Q8EEB1
B	399	HIS	-	expression tag	UNP Q8EEB1
B	400	HIS	-	expression tag	UNP Q8EEB1
B	401	HIS	-	expression tag	UNP Q8EEB1
B	402	HIS	-	expression tag	UNP Q8EEB1
B	403	HIS	-	expression tag	UNP Q8EEB1
C	396	LEU	-	expression tag	UNP Q8EEB1
C	397	GLU	-	expression tag	UNP Q8EEB1
C	398	HIS	-	expression tag	UNP Q8EEB1
C	399	HIS	-	expression tag	UNP Q8EEB1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	400	HIS	-	expression tag	UNP Q8EEB1
C	401	HIS	-	expression tag	UNP Q8EEB1
C	402	HIS	-	expression tag	UNP Q8EEB1
C	403	HIS	-	expression tag	UNP Q8EEB1
D	396	LEU	-	expression tag	UNP Q8EEB1
D	397	GLU	-	expression tag	UNP Q8EEB1
D	398	HIS	-	expression tag	UNP Q8EEB1
D	399	HIS	-	expression tag	UNP Q8EEB1
D	400	HIS	-	expression tag	UNP Q8EEB1
D	401	HIS	-	expression tag	UNP Q8EEB1
D	402	HIS	-	expression tag	UNP Q8EEB1
D	403	HIS	-	expression tag	UNP Q8EEB1

- Molecule 2 is N-({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-D-GLUTAMIC ACID (three-letter code: PDG) (formula: C₁₃H₁₉N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	A	2	Total 2	Cl 2	0	0
3	D	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Na 1	0	0

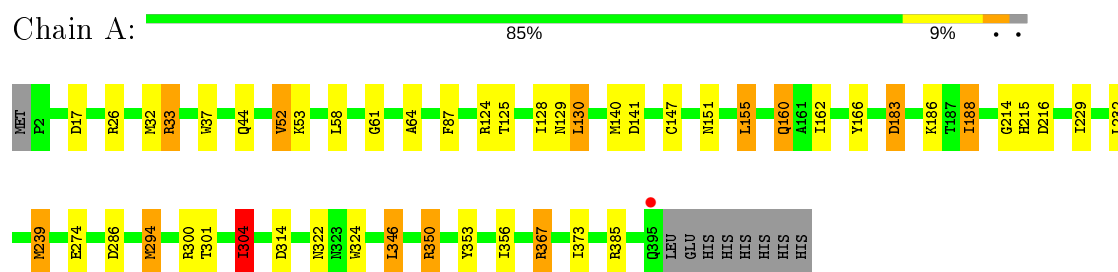
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total 205	O 205	0	0
5	B	183	Total 183	O 183	0	0
5	C	142	Total 142	O 142	0	0
5	D	180	Total 180	O 180	0	0

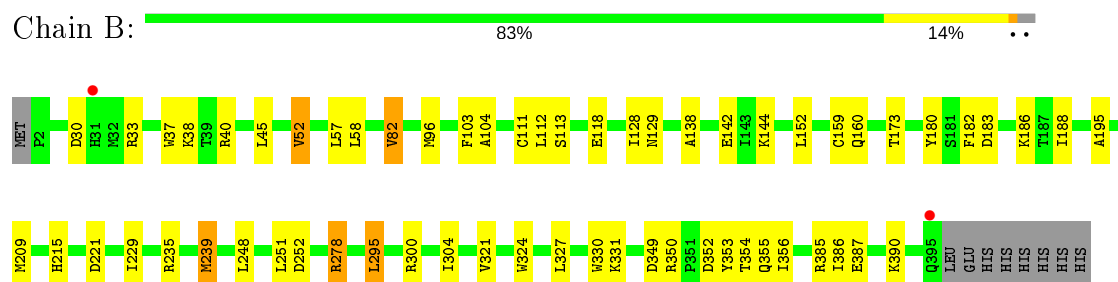
3 Residue-property plots [i](#)

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.

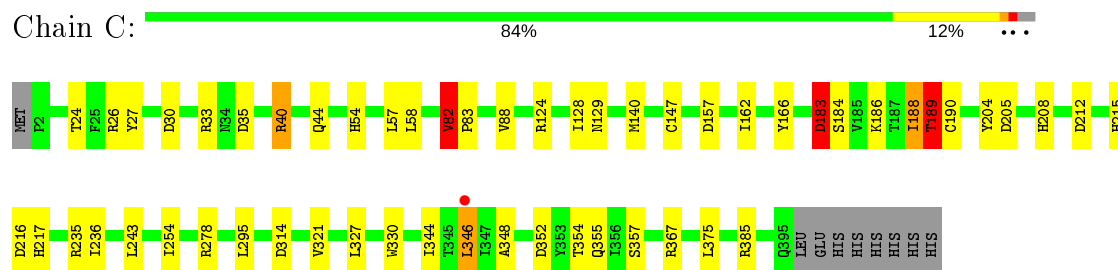
- Molecule 1: 8-amino-3,8-dideoxy-alpha-D-manno-octulosonate transaminase



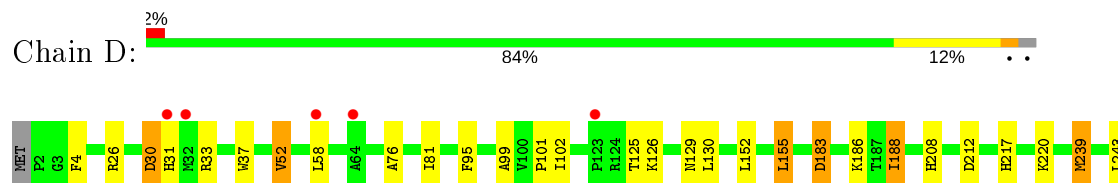
- Molecule 1: 8-amino-3,8-dideoxy-alpha-D-manno-octulosonate transaminase

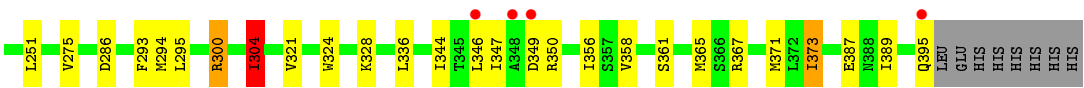


- Molecule 1: 8-amino-3,8-dideoxy-alpha-D-manno-octulosonate transaminase



- Molecule 1: 8-amino-3,8-dideoxy-alpha-D-manno-octulosonate transaminase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	266.63Å 61.67Å 99.64Å 90.00° 102.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 29.52 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-2.15) 95.9 (29.52-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.171 , 0.226 0.179 , 0.229	Depositor DCC
R_{free} test set	4100 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13031	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: PDG, NA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/3120	1.11	24/4214 (0.6%)
1	B	0.54	0/3119	1.12	16/4213 (0.4%)
1	C	0.53	0/3120	1.09	22/4214 (0.5%)
1	D	0.54	0/3120	1.08	12/4214 (0.3%)
All	All	0.55	0/12479	1.10	74/16855 (0.4%)

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

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ARG	NE-CZ-NH1	14.43	127.51	120.30
1	B	278	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	C	205	ASP	CB-CG-OD1	11.38	128.54	118.30
1	C	40	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	C	205	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	B	239	MET	CA-CB-CG	7.63	126.28	113.30
1	A	141	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	142	GLU	OE1-CD-OE2	7.43	132.21	123.30
1	B	239	MET	CG-SD-CE	-7.41	88.35	100.20
1	B	82	VAL	CB-CA-C	-7.39	97.35	111.40
1	A	183	ASP	CB-CG-OD2	7.21	124.79	118.30
1	D	286	ASP	CB-CG-OD2	-7.15	111.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ILE	CG1-CB-CG2	-7.08	95.83	111.40
1	D	26	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	C	183	ASP	CB-CG-OD2	6.88	124.49	118.30
1	A	367	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	C	82	VAL	CB-CA-C	-6.67	98.73	111.40
1	A	373	ILE	CG1-CB-CG2	-6.63	96.81	111.40
1	A	314	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	33	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	314	ASP	CB-CG-OD2	6.45	124.11	118.30
1	D	183	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	286	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	C	295	LEU	CA-CB-CG	-6.29	100.82	115.30
1	C	385	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	52	VAL	CB-CA-C	-6.29	99.45	111.40
1	D	304	ILE	CG1-CB-CG2	-6.28	97.58	111.40
1	C	33	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	385	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	300	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	B	235	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	26	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	C	367	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	286	ASP	CB-CG-OD1	6.18	123.86	118.30
1	D	155	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	216	ASP	CB-CG-OD2	6.16	123.85	118.30
1	A	155	LEU	CA-CB-CG	6.12	129.37	115.30
1	D	239	MET	CG-SD-CE	-6.11	90.42	100.20
1	C	35	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	33	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	157	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	C	235	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	385	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	40	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	155	LEU	CB-CG-CD1	5.85	120.94	111.00
1	B	252	ASP	CB-CG-OD2	5.84	123.56	118.30
1	C	367	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	C	124	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	346	LEU	CA-CB-CG	5.70	128.40	115.30
1	C	189	THR	CB-CA-C	-5.68	96.27	111.60
1	A	130	LEU	CB-CG-CD2	5.62	120.55	111.00
1	A	350	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	274	GLU	CB-CA-C	-5.60	99.20	110.40
1	A	239	MET	CA-CB-CG	5.57	122.77	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	VAL	CB-CA-C	-5.54	100.88	111.40
1	B	239	MET	N-CA-CB	5.50	120.50	110.60
1	B	278	ARG	CD-NE-CZ	5.39	131.14	123.60
1	C	278	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	D	373	ILE	CG1-CB-CG2	-5.30	99.73	111.40
1	C	30	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	17	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	180	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	D	365	MET	CG-SD-CE	-5.26	91.79	100.20
1	A	141	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	D	300	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	B	160	GLN	CB-CA-C	-5.17	100.07	110.40
1	C	216	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	160	GLN	CB-CA-C	-5.13	100.14	110.40
1	C	216	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	D	350	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	367	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	26	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	295	LEU	CA-CB-CG	-5.05	103.68	115.30
1	C	26	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	349	ASP	Peptide

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3054	0	3030	23	0
1	B	3053	0	3030	31	0
1	C	3054	0	3030	28	0
1	D	3054	0	3030	28	0
2	A	25	0	14	6	0
2	B	25	0	14	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	25	0	14	7	0
2	D	25	0	15	7	0
3	A	2	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	1	0	0	0	0
5	A	205	0	0	1	0
5	B	183	0	0	1	0
5	C	142	0	0	0	0
5	D	180	0	0	1	0
All	All	13031	0	12177	103	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 4.

All (103) 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:B:186:LYS:NZ	2:B:501:PDG:HNA	1.30	1.25
1:B:186:LYS:NZ	2:B:501:PDG:NA	1.89	1.18
1:C:162:ILE:HD13	1:C:188:ILE:HD11	1.58	0.85
1:B:188:ILE:HD12	1:B:251:LEU:HD13	1.63	0.81
1:A:162:ILE:HD13	1:A:188:ILE:HD11	1.64	0.80
1:C:184:SER:HA	1:C:189:THR:CG2	2.15	0.77
1:C:184:SER:HA	1:C:189:THR:HG21	1.68	0.75
1:A:322:ASN:HB3	3:A:502:CL:CL	2.25	0.72
1:B:186:LYS:HZ1	2:B:501:PDG:HNA	0.72	0.71
1:C:186:LYS:NZ	2:C:501:PDG:NA	2.39	0.70
1:D:387:GLU:OE1	5:D:601:HOH:O	2.10	0.70
1:C:186:LYS:CE	2:C:501:PDG:H4A2	2.23	0.68
1:C:186:LYS:HE2	2:C:501:PDG:H4A2	1.75	0.68
1:B:188:ILE:HD11	1:B:251:LEU:HB2	1.75	0.68
1:D:186:LYS:NZ	2:D:501:PDG:NA	2.44	0.64
1:B:188:ILE:CD1	1:B:251:LEU:HD13	2.26	0.64
1:A:353:TYR:HA	1:A:356:ILE:HD11	1.81	0.62
1:B:45:LEU:HD23	1:B:248:LEU:HD23	1.82	0.61
1:D:186:LYS:HZ1	2:D:501:PDG:HNA	1.47	0.61
1:D:188:ILE:HD12	1:D:251:LEU:HD13	1.81	0.61
1:A:128:ILE:HD12	1:A:147:CYS:SG	2.41	0.60
1:A:186:LYS:CE	2:A:501:PDG:H4A2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LYS:HE2	2:D:501:PDG:H4A2	1.84	0.59
1:A:353:TYR:HA	1:A:356:ILE:CD1	2.34	0.58
1:A:87:PHE:CZ	2:A:501:PDG:HGA2	2.41	0.56
1:A:186:LYS:NZ	2:A:501:PDG:NA	2.55	0.54
1:A:232:LEU:HD21	1:B:96:MET:HG3	1.91	0.53
1:A:294:MET:HA	1:A:367:ARG:O	2.08	0.53
1:D:208:HIS:ND1	1:D:217:HIS:HD2	2.07	0.53
1:B:128:ILE:CD1	1:B:152:LEU:HD13	2.39	0.52
1:D:186:LYS:CE	2:D:501:PDG:H4A2	2.38	0.52
1:D:371:MET:HE1	1:D:389:ILE:HD11	1.90	0.52
1:D:212:ASP:OD2	1:D:217:HIS:HE1	1.92	0.52
1:B:221:ASP:HB2	5:B:735:HOH:O	2.10	0.52
1:C:140:MET:HB2	1:C:166:TYR:CE1	2.46	0.51
1:B:128:ILE:HD11	1:B:152:LEU:HD13	1.93	0.50
1:A:214:GLY:HA3	1:A:229:ILE:O	2.10	0.50
1:A:186:LYS:HE2	2:A:501:PDG:H4A2	1.93	0.49
1:D:186:LYS:NZ	2:D:501:PDG:HNA	2.03	0.49
1:D:300:ARG:CZ	1:D:304:ILE:HD11	2.42	0.48
1:C:254:ILE:HG23	1:C:375:LEU:HD11	1.94	0.48
1:A:140:MET:HB2	1:A:166:TYR:CE1	2.48	0.48
1:C:27:TYR:CE1	1:C:217:HIS:CE1	3.00	0.48
1:C:208:HIS:ND1	1:C:217:HIS:HD2	2.12	0.48
1:B:386:ILE:HG22	1:B:390:LYS:HE2	1.96	0.48
1:C:54:HIS:HB3	1:C:204:TYR:CD1	2.49	0.48
1:B:57:LEU:HD12	1:B:195:ALA:HB2	1.96	0.47
1:B:182:PHE:CD2	1:B:188:ILE:HG22	2.49	0.47
1:C:128:ILE:HD12	1:C:147:CYS:SG	2.55	0.47
1:A:301:THR:OG1	1:A:367:ARG:HA	2.14	0.47
1:D:344:ILE:HD12	1:D:347:ILE:HD12	1.97	0.47
1:A:215:HIS:CE1	1:B:324:TRP:CZ2	3.02	0.47
1:B:103:PHE:CD2	1:B:356:ILE:HD13	2.50	0.46
1:C:352:ASP:OD1	1:C:354:THR:OG1	2.23	0.46
1:D:30:ASP:OD1	1:D:30:ASP:N	2.48	0.46
1:C:24:THR:HG21	1:D:243:LEU:HD21	1.98	0.46
1:B:186:LYS:CE	2:B:501:PDG:NA	2.77	0.46
1:C:212:ASP:OD2	1:C:217:HIS:HE1	1.98	0.46
1:B:295:LEU:HD22	1:B:304:ILE:HG13	1.99	0.45
1:A:215:HIS:CD2	1:B:324:TRP:CH2	3.05	0.45
1:A:33:ARG:HD3	1:A:37:TRP:CZ2	2.52	0.45
1:C:183:ASP:O	1:C:189:THR:HG23	2.17	0.44
1:B:188:ILE:HD11	1:B:251:LEU:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LYS:HZ3	2:C:501:PDG:CAA	2.31	0.44
1:C:186:LYS:HZ1	2:C:501:PDG:HNA	1.66	0.44
1:D:358:VAL:HB	1:D:361:SER:HB2	1.99	0.44
1:C:82:VAL:HG12	1:C:83:PRO:HD2	2.00	0.44
1:B:327:LEU:HA	1:B:330:TRP:CE3	2.52	0.43
1:C:190:CYS:C	1:C:243:LEU:HD23	2.39	0.43
1:A:160:GLN:HG3	2:A:501:PDG:H2A1	2.01	0.43
1:D:186:LYS:CE	2:D:501:PDG:NA	2.82	0.43
1:D:33:ARG:HD3	1:D:37:TRP:CE2	2.53	0.43
1:D:95:PHE:CZ	1:D:336:LEU:HD21	2.53	0.43
1:A:61:GLY:O	1:A:64:ALA:HB3	2.18	0.43
1:B:186:LYS:CE	2:B:501:PDG:HNA	2.21	0.43
1:C:186:LYS:CE	2:C:501:PDG:C4A	2.93	0.43
1:C:327:LEU:HA	1:C:330:TRP:CE3	2.53	0.43
1:D:300:ARG:CZ	1:D:304:ILE:CD1	2.96	0.43
1:A:186:LYS:HZ3	2:A:501:PDG:CBA	2.31	0.42
1:D:99:ALA:O	1:D:344:ILE:HD13	2.19	0.42
1:B:209:MET:HE3	1:B:229:ILE:HG12	2.01	0.42
1:A:125:THR:OG1	5:A:601:HOH:O	2.20	0.42
1:B:352:ASP:OD2	1:B:354:THR:OG1	2.36	0.42
1:D:300:ARG:NH1	1:D:304:ILE:HD11	2.34	0.42
1:C:344:ILE:O	1:C:344:ILE:HG13	2.20	0.42
1:A:324:TRP:CZ2	1:B:215:HIS:CE1	3.07	0.42
1:C:346:LEU:CD1	1:D:76:ALA:HB1	2.51	0.41
1:B:159:CYS:HB2	2:B:501:PDG:C2	2.50	0.41
1:B:52:VAL:HG13	1:B:173:THR:HG22	2.01	0.41
1:B:37:TRP:HB3	1:B:40:ARG:HB3	2.03	0.41
1:D:81:ILE:HA	1:D:102:ILE:O	2.21	0.41
1:C:215:HIS:CE1	1:D:324:TRP:CZ2	3.09	0.41
1:C:140:MET:HB2	1:C:166:TYR:CD1	2.55	0.41
1:D:125:THR:HG22	1:D:152:LEU:HD22	2.03	0.41
1:D:275:VAL:HG13	1:D:293:PHE:HB2	2.03	0.41
1:D:186:LYS:CE	2:D:501:PDG:C4A	2.98	0.41
1:D:95:PHE:CE1	1:D:101:PRO:HD2	2.56	0.41
1:A:300:ARG:CZ	1:A:304:ILE:HD13	2.52	0.40
1:B:353:TYR:HD1	1:B:356:ILE:HD11	1.86	0.40
1:C:186:LYS:HZ3	2:C:501:PDG:CBA	2.35	0.40
1:B:111:CYS:HB2	1:B:138:ALA:HB2	2.04	0.40
1:B:104:ALA:HB3	1:B:112:LEU:HD22	2.03	0.40
1:C:57:LEU:HD23	1:C:236:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	393/403 (98%)	381 (97%)	12 (3%)	0	100	100
1	B	393/403 (98%)	380 (97%)	12 (3%)	1 (0%)	41	37
1	C	393/403 (98%)	380 (97%)	12 (3%)	1 (0%)	41	37
1	D	393/403 (98%)	377 (96%)	15 (4%)	1 (0%)	41	37
All	All	1572/1612 (98%)	1518 (97%)	51 (3%)	3 (0%)	47	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	348	ALA
1	D	31	HIS
1	B	350	ARG

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	325/333 (98%)	308 (95%)	17 (5%)	23	19
1	B	325/333 (98%)	309 (95%)	16 (5%)	25	21
1	C	325/333 (98%)	312 (96%)	13 (4%)	31	29
1	D	325/333 (98%)	303 (93%)	22 (7%)	16	10
All	All	1300/1332 (98%)	1232 (95%)	68 (5%)	23	19

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	44	GLN
1	A	52	VAL
1	A	53	LYS
1	A	58	LEU
1	A	124	ARG
1	A	129	ASN
1	A	130	LEU
1	A	151	ASN
1	A	155	LEU
1	A	183	ASP
1	A	188	ILE
1	A	239	MET
1	A	294	MET
1	A	304	ILE
1	A	346	LEU
1	A	350	ARG
1	B	30	ASP
1	B	38	LYS
1	B	52	VAL
1	B	58	LEU
1	B	82	VAL
1	B	113	SER
1	B	118	GLU
1	B	129	ASN
1	B	144	LYS
1	B	183	ASP
1	B	239	MET
1	B	278	ARG
1	B	321	VAL
1	B	331	LYS
1	B	355	GLN
1	B	387	GLU
1	C	40	ARG
1	C	44	GLN
1	C	58	LEU
1	C	82	VAL
1	C	88	VAL
1	C	129	ASN
1	C	183	ASP
1	C	188	ILE
1	C	189	THR
1	C	321	VAL

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Mol	Chain	Res	Type
1	C	346	LEU
1	C	355	GLN
1	C	357	SER
1	D	4	PHE
1	D	30	ASP
1	D	52	VAL
1	D	58	LEU
1	D	126	LYS
1	D	129	ASN
1	D	130	LEU
1	D	155	LEU
1	D	183	ASP
1	D	188	ILE
1	D	220	LYS
1	D	239	MET
1	D	294	MET
1	D	295	LEU
1	D	304	ILE
1	D	321	VAL
1	D	328	LYS
1	D	346	LEU
1	D	349	ASP
1	D	356	ILE
1	D	373	ILE
1	D	395	GLN

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

Mol	Chain	Res	Type
1	A	28	ASN
1	A	44	GLN
1	C	151	ASN
1	C	217	HIS
1	C	355	GLN
1	D	28	ASN
1	D	150	HIS
1	D	151	ASN
1	D	217	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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$
2	PDG	D	501	-	19,25,25	2.17	3 (15%)	24,35,35	2.62	9 (37%)
2	PDG	A	501	-	19,25,25	2.20	3 (15%)	24,35,35	2.61	9 (37%)
2	PDG	C	501	-	19,25,25	2.17	3 (15%)	24,35,35	2.70	10 (41%)
2	PDG	B	501	-	19,25,25	2.96	9 (47%)	24,35,35	2.22	7 (29%)

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
2	PDG	D	501	-	-	10/14/20/20	0/1/1/1
2	PDG	A	501	-	-	10/14/20/20	0/1/1/1
2	PDG	C	501	-	-	8/14/20/20	0/1/1/1
2	PDG	B	501	-	-	7/14/20/20	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PDG	C3-C2	8.83	1.49	1.40
2	A	501	PDG	C3-C2	6.05	1.47	1.40
2	C	501	PDG	C3-C2	6.04	1.46	1.40
2	D	501	PDG	C3-C2	5.87	1.46	1.40
2	A	501	PDG	C5-C4	5.47	1.48	1.40
2	D	501	PDG	C3-C4	4.86	1.47	1.40
2	C	501	PDG	C3-C4	4.73	1.47	1.40
2	D	501	PDG	C5-C4	4.73	1.47	1.40
2	C	501	PDG	C5-C4	4.46	1.46	1.40
2	A	501	PDG	C3-C4	3.96	1.46	1.40
2	B	501	PDG	O3-C3	-3.93	1.27	1.37
2	B	501	PDG	C5-C4	3.83	1.45	1.40
2	B	501	PDG	P-OP2	-3.68	1.40	1.54
2	B	501	PDG	P-OP3	-3.42	1.41	1.54
2	B	501	PDG	P-OP1	-2.67	1.41	1.50
2	B	501	PDG	P-OP4	-2.38	1.52	1.60
2	B	501	PDG	CAA-NA	-2.37	1.43	1.47
2	B	501	PDG	C3-C4	2.23	1.43	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PDG	C4A-NA-CAA	7.00	127.27	113.83
2	C	501	PDG	C4A-NA-CAA	6.91	127.10	113.83
2	D	501	PDG	CGA-CBA-CAA	-6.72	99.46	113.04
2	A	501	PDG	CGA-CBA-CAA	-6.41	100.09	113.04
2	D	501	PDG	C4A-NA-CAA	5.81	125.00	113.83
2	C	501	PDG	C4A-C4-C3	5.71	126.15	120.04
2	B	501	PDG	C4A-C4-C3	5.14	125.55	120.04
2	B	501	PDG	CGA-CBA-CAA	-4.89	103.16	113.04
2	A	501	PDG	C4A-C4-C3	4.86	125.25	120.04
2	C	501	PDG	OP2-P-OP4	-4.37	95.10	106.73
2	D	501	PDG	C4A-C4-C3	4.22	124.56	120.04
2	C	501	PDG	OP4-C5A-C5	4.17	117.30	109.35
2	B	501	PDG	C3-C4-C5	-4.00	114.88	118.72
2	D	501	PDG	C6-N1-C2	3.87	126.34	119.17
2	D	501	PDG	C4A-C4-C5	-3.70	115.60	119.71
2	B	501	PDG	C4-C4A-NA	3.65	121.82	111.78
2	C	501	PDG	OP2-P-OP1	3.46	124.24	110.68
2	C	501	PDG	CGA-CBA-CAA	-3.34	106.29	113.04
2	A	501	PDG	C6-N1-C2	3.01	124.75	119.17
2	B	501	PDG	OP4-C5A-C5	2.64	114.39	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PDG	C5A-C5-C6	2.52	123.52	119.37
2	B	501	PDG	O3-C3-C2	2.48	122.90	117.49
2	B	501	PDG	C6-C5-C4	2.48	119.87	118.12
2	C	501	PDG	C4A-C4-C5	-2.40	117.04	119.71
2	A	501	PDG	OP3-P-OP2	2.36	116.64	107.64
2	A	501	PDG	C4A-C4-C5	-2.35	117.10	119.71
2	A	501	PDG	C2A-C2-N1	2.32	122.21	117.67
2	C	501	PDG	C3-C4-C5	-2.24	116.57	118.72
2	D	501	PDG	C6-C5-C4	-2.21	116.56	118.12
2	A	501	PDG	C3-C2-N1	-2.15	117.99	120.77
2	D	501	PDG	C4-C3-C2	-2.08	116.87	120.06
2	D	501	PDG	C5A-C5-C6	2.03	122.72	119.37
2	D	501	PDG	C3-C2-N1	-2.02	118.16	120.77
2	A	501	PDG	OP4-C5A-C5	2.01	113.18	109.35
2	C	501	PDG	C6-N1-C2	2.01	122.88	119.17

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PDG	C5-C4-C4A-NA
2	B	501	PDG	CBA-CAA-NA-C4A
2	B	501	PDG	CA-CAA-NA-C4A
2	B	501	PDG	CA-CAA-CBA-CGA
2	D	501	PDG	C5A-OP4-P-OP2
2	D	501	PDG	C5A-OP4-P-OP3
2	D	501	PDG	NA-CAA-CBA-CGA
2	D	501	PDG	CA-CAA-CBA-CGA
2	A	501	PDG	C5A-OP4-P-OP1
2	A	501	PDG	C5A-OP4-P-OP3
2	A	501	PDG	NA-CAA-CBA-CGA
2	A	501	PDG	CA-CAA-CBA-CGA
2	C	501	PDG	C5A-OP4-P-OP2
2	C	501	PDG	C5A-OP4-P-OP3
2	B	501	PDG	NA-CAA-CBA-CGA
2	D	501	PDG	C5-C4-C4A-NA
2	A	501	PDG	C5-C4-C4A-NA
2	C	501	PDG	C5-C4-C4A-NA
2	D	501	PDG	C4-C4A-NA-CAA
2	A	501	PDG	C4-C4A-NA-CAA
2	C	501	PDG	C4-C4A-NA-CAA
2	B	501	PDG	C4-C4A-NA-CAA

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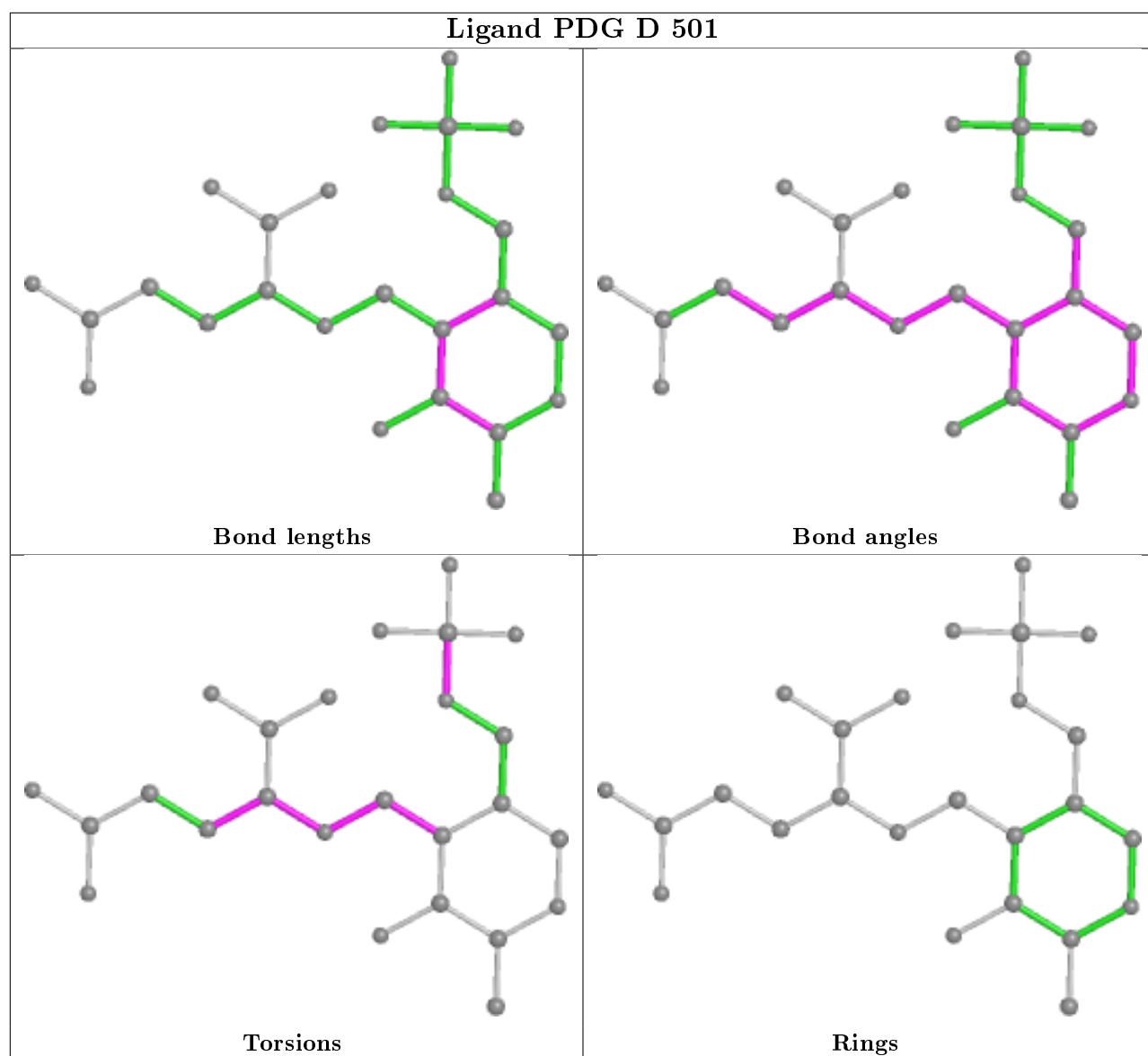
Mol	Chain	Res	Type	Atoms
2	D	501	PDG	C3-C4-C4A-NA
2	A	501	PDG	C3-C4-C4A-NA
2	C	501	PDG	C3-C4-C4A-NA
2	A	501	PDG	CBA-CAA-NA-C4A
2	A	501	PDG	C5A-OP4-P-OP2
2	D	501	PDG	C5A-OP4-P-OP1
2	C	501	PDG	NA-CAA-CBA-CGA
2	D	501	PDG	CBA-CAA-NA-C4A
2	D	501	PDG	CA-CAA-NA-C4A
2	A	501	PDG	CA-CAA-NA-C4A
2	C	501	PDG	CA-CAA-NA-C4A
2	B	501	PDG	C3-C4-C4A-NA
2	C	501	PDG	C5A-OP4-P-OP1

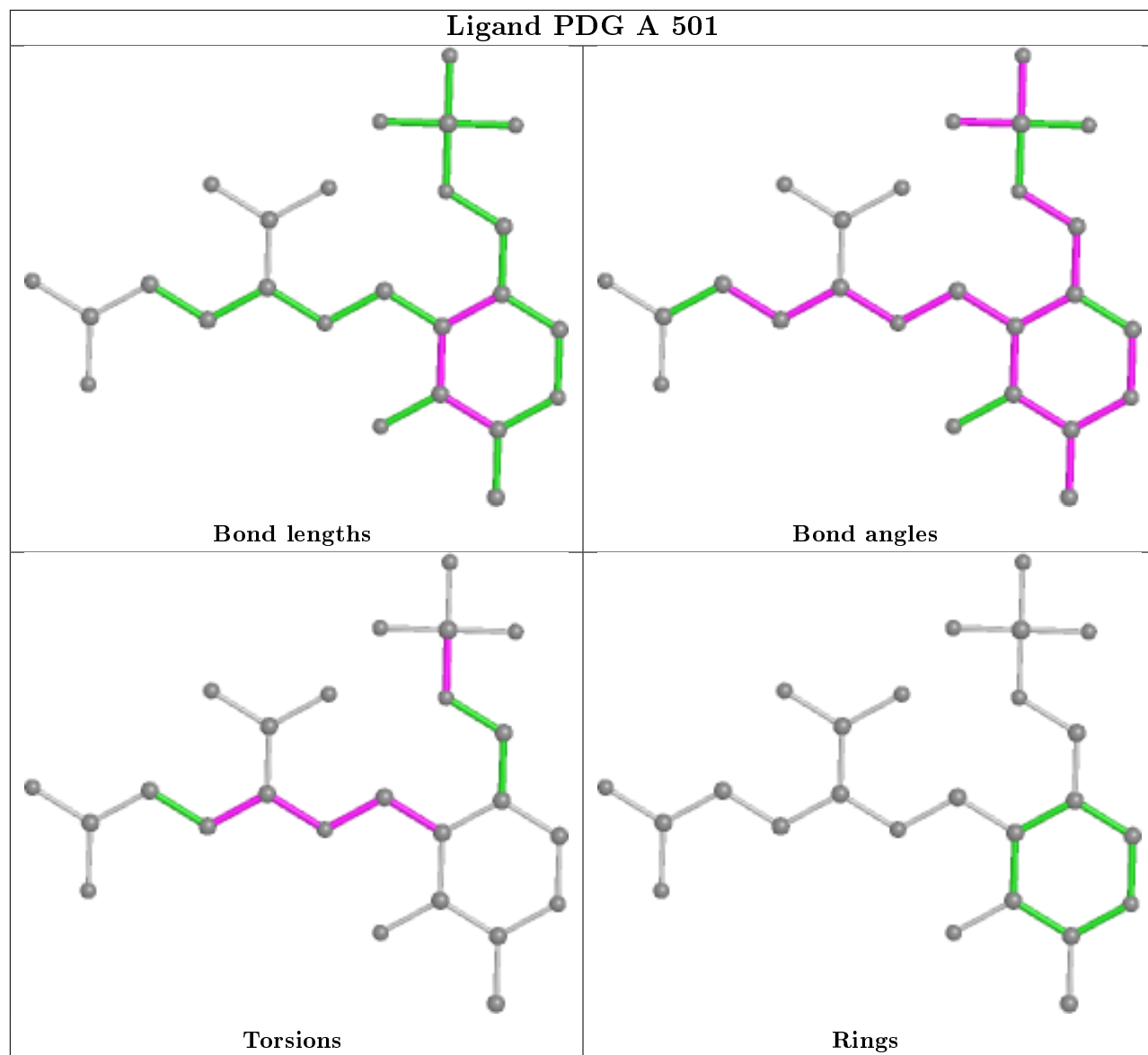
There are no ring outliers.

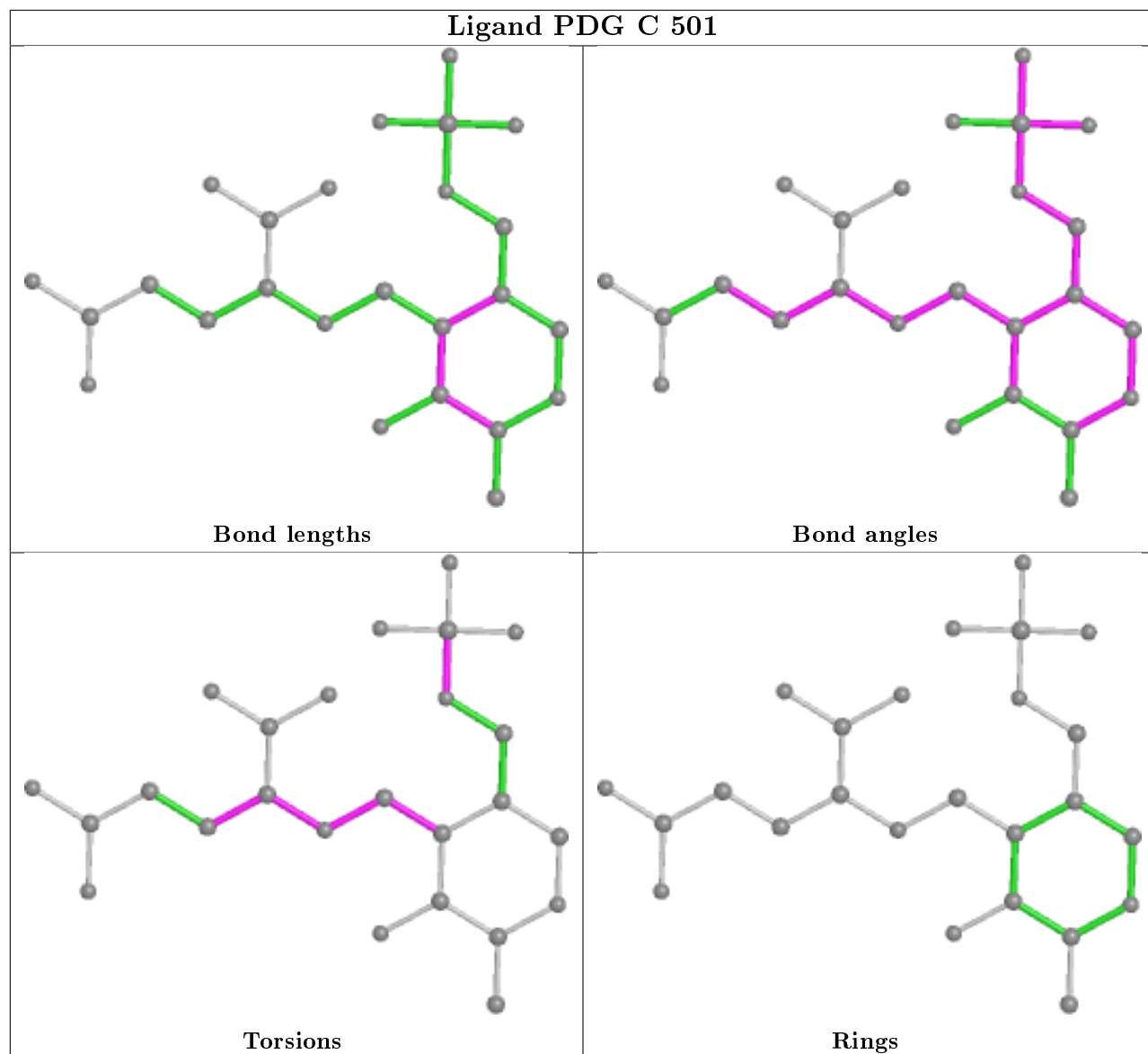
4 monomers are involved in 26 short contacts:

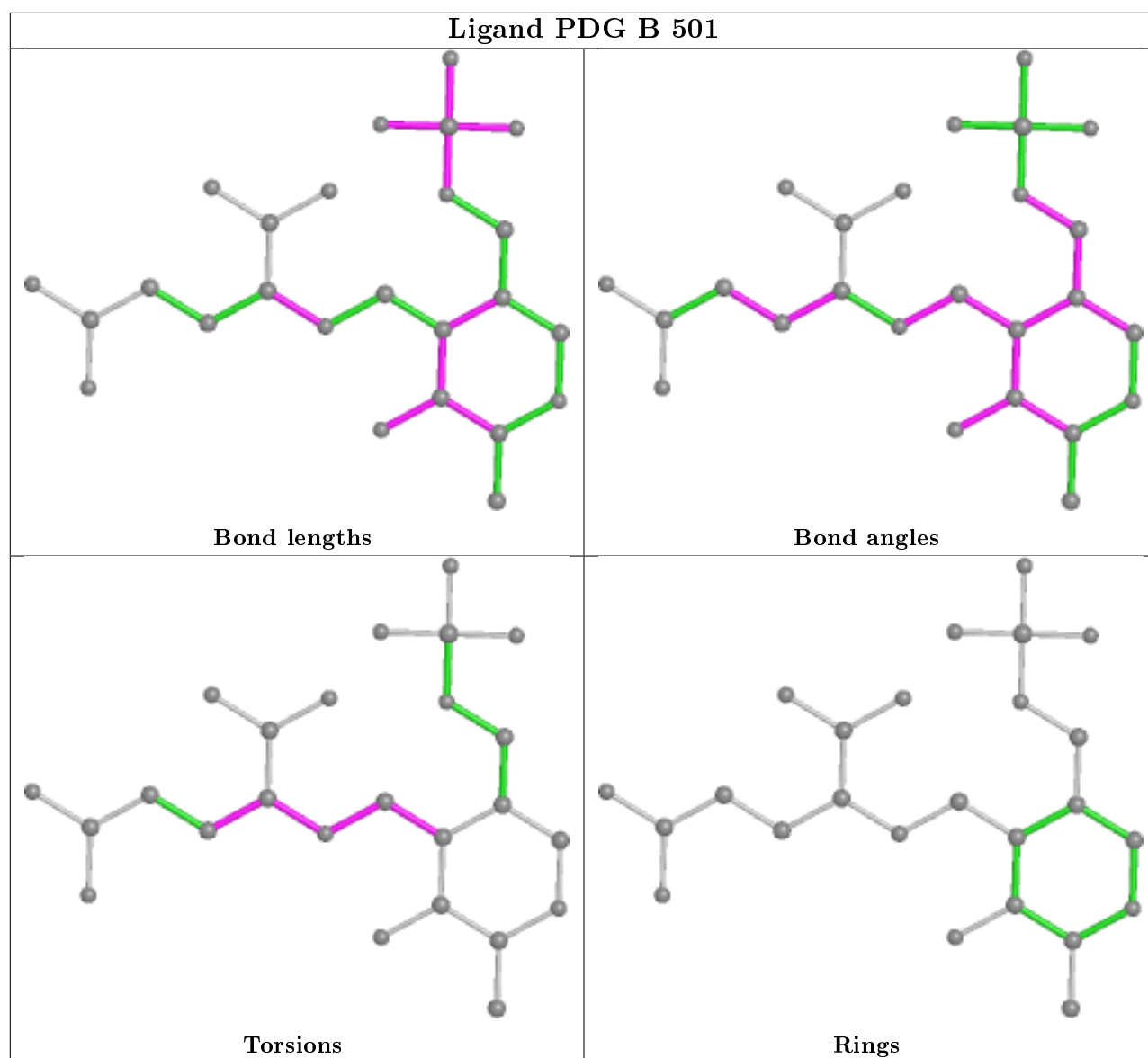
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PDG	7	0
2	A	501	PDG	6	0
2	C	501	PDG	7	0
2	B	501	PDG	6	0

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	394/403 (97%)	-0.32	1 (0%) 94 95	11, 18, 34, 59	0
1	B	394/403 (97%)	-0.21	2 (0%) 91 93	12, 20, 38, 71	0
1	C	394/403 (97%)	-0.17	1 (0%) 94 95	12, 22, 42, 66	0
1	D	394/403 (97%)	-0.17	9 (2%) 60 68	11, 21, 40, 72	0
All	All	1576/1612 (97%)	-0.22	13 (0%) 86 89	11, 20, 39, 72	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	395	GLN	4.0
1	D	395	GLN	3.1
1	D	123	PRO	3.0
1	D	346	LEU	2.6
1	B	31	HIS	2.6
1	D	348	ALA	2.6
1	D	349	ASP	2.5
1	D	64	ALA	2.5
1	A	395	GLN	2.5
1	C	346	LEU	2.4
1	D	31	HIS	2.2
1	D	32	MET	2.2
1	D	58	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

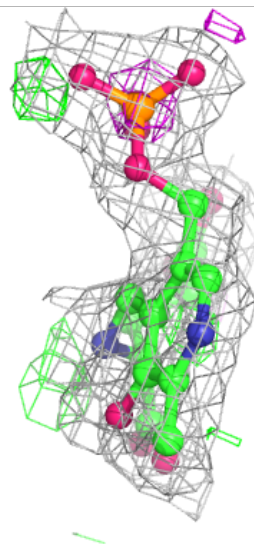
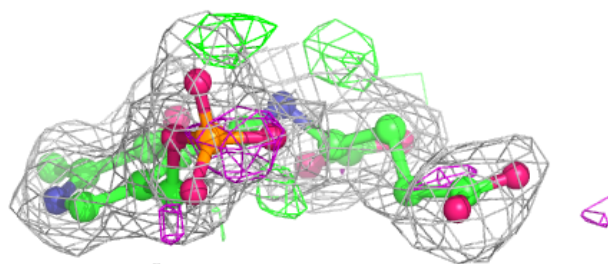
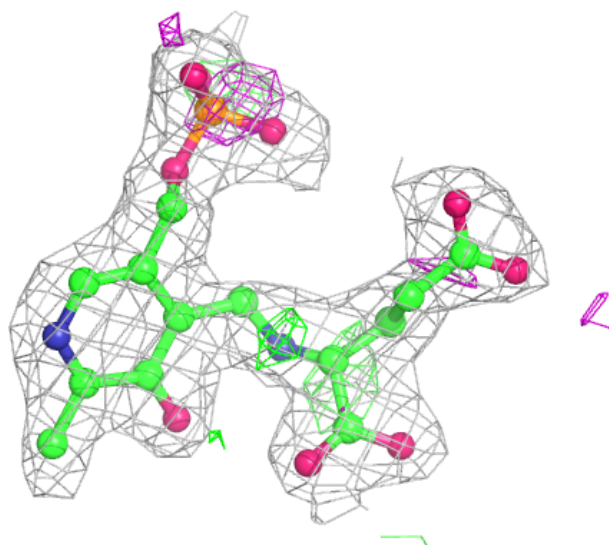
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	C	502	1/1	0.93	0.07	37,37,37,37	0
2	PDG	B	501	25/25	0.95	0.13	9,17,27,30	0
2	PDG	C	501	25/25	0.97	0.15	10,17,24,27	0
2	PDG	D	501	25/25	0.97	0.13	10,16,22,25	0
3	CL	A	502	1/1	0.98	0.06	25,25,25,25	0
2	PDG	A	501	25/25	0.98	0.12	10,15,20,25	0
3	CL	D	502	1/1	0.99	0.03	16,16,16,16	0
3	CL	A	503	1/1	0.99	0.08	17,17,17,17	0
3	CL	C	503	1/1	1.00	0.04	15,15,15,15	0
3	CL	B	502	1/1	1.00	0.06	17,17,17,17	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.

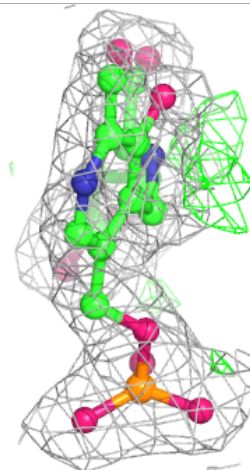
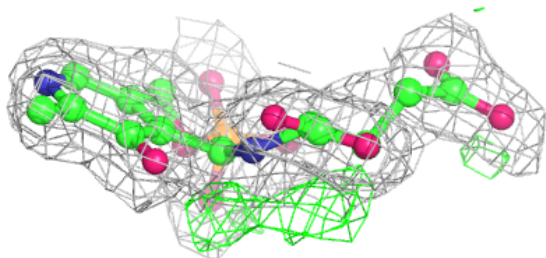
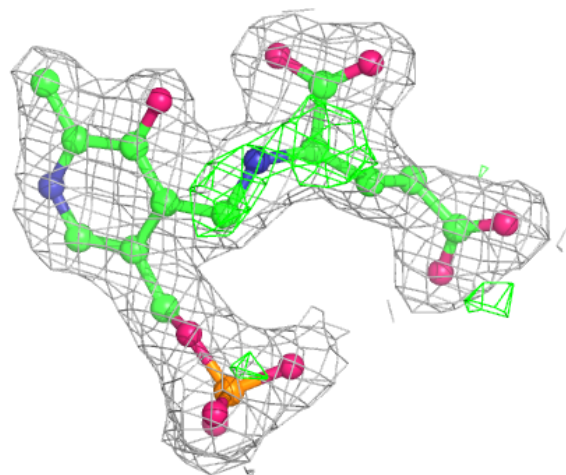
Electron density around PDG B 501:

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



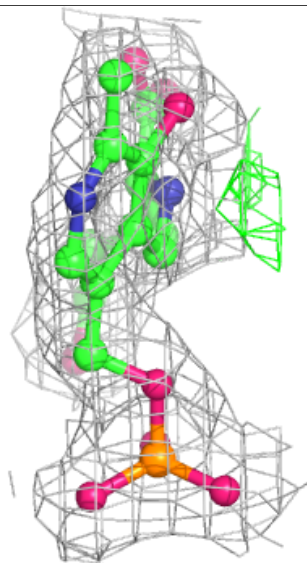
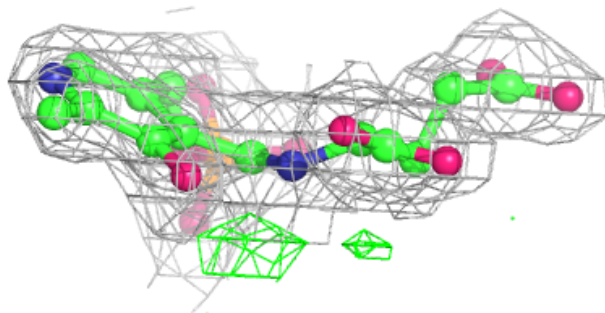
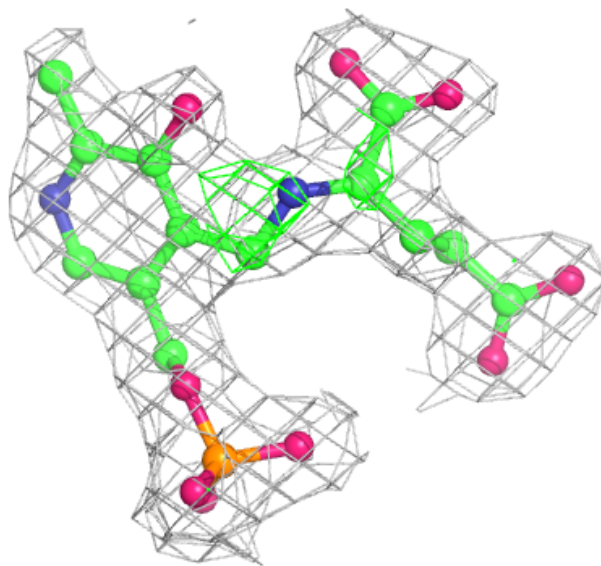
Electron density around PDG C 501:

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



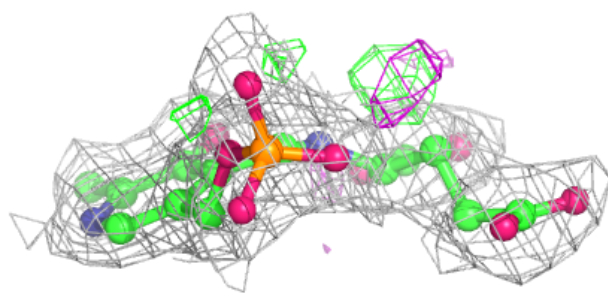
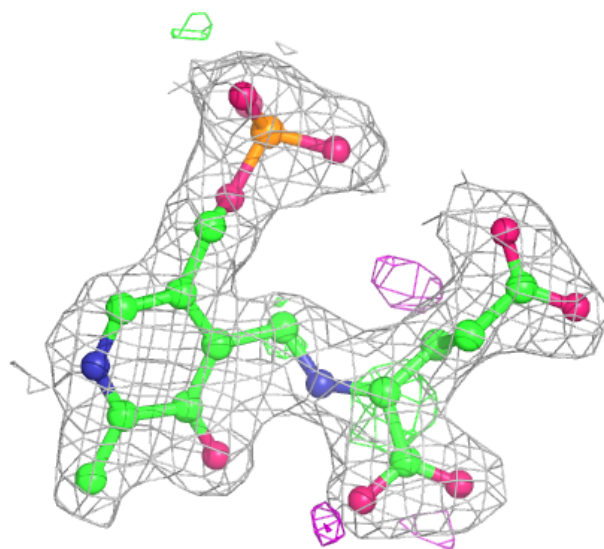
Electron density around PDG D 501:

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



Electron density around PDG A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.