



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:41 PM UTC

PDB ID : 7A20 / pdb_00007a20
Title : Azobenzene-Based Inhibitors for Tryptophan Synthase
Authors : Rajendran, C.; Sterner, R.
Deposited on : 2020-08-14
Resolution : 2.50 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:

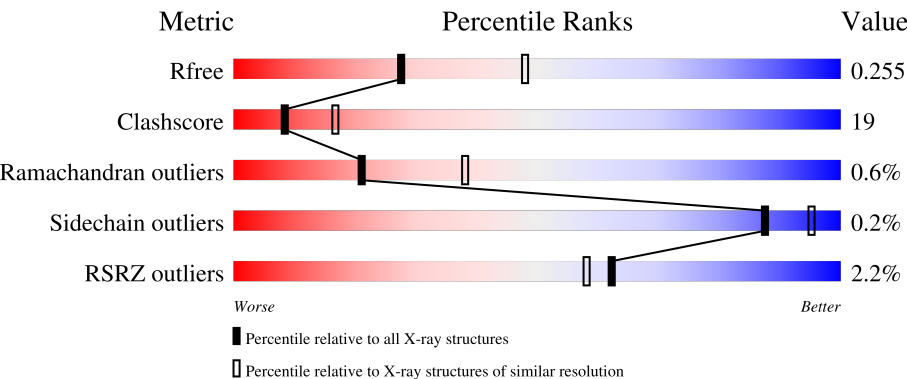
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	709	% 23% 13% 64%
1	B	709	% 39% 16% 45%
1	C	709	% 22% 13% 65%
1	D	709	% 42% 13% 44%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	144	B	502	-	-	X	-
3	144	D	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9806 atoms, of which 12 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 Tryptophan synthase alpha chain,Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1919	1228	330	353	8			
1	B	390	Total	C	N	O	S	0	0	0
			2954	1858	517	560	19			
1	C	249	Total	C	N	O	S	0	1	0
			1876	1194	322	352	8			
1	D	394	Total	C	N	O	S	0	1	0
			2982	1872	526	565	19			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	SER	-	expression tag	UNP A0A0D6FWC1
A	-24	THR	-	expression tag	UNP A0A0D6FWC1
A	-23	THR	-	expression tag	UNP A0A0D6FWC1
A	-22	ARG	-	expression tag	UNP A0A0D6FWC1
A	-21	PRO	-	expression tag	UNP A0A0D6FWC1
A	-20	ALA	-	expression tag	UNP A0A0D6FWC1
A	-19	MET	-	expression tag	UNP A0A0D6FWC1
A	-18	GLY	-	expression tag	UNP A0A0D6FWC1
A	-17	SER	-	expression tag	UNP A0A0D6FWC1
A	-16	SER	-	expression tag	UNP A0A0D6FWC1
A	-15	HIS	-	expression tag	UNP A0A0D6FWC1
A	-14	HIS	-	expression tag	UNP A0A0D6FWC1
A	-13	HIS	-	expression tag	UNP A0A0D6FWC1
A	-12	HIS	-	expression tag	UNP A0A0D6FWC1
A	-11	HIS	-	expression tag	UNP A0A0D6FWC1
A	-10	HIS	-	expression tag	UNP A0A0D6FWC1
A	-9	SER	-	expression tag	UNP A0A0D6FWC1
A	-8	SER	-	expression tag	UNP A0A0D6FWC1
A	-7	GLY	-	expression tag	UNP A0A0D6FWC1
A	-6	LEU	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP A0A0D6FWC1
A	-4	PRO	-	expression tag	UNP A0A0D6FWC1
A	-3	ARG	-	expression tag	UNP A0A0D6FWC1
A	-2	GLY	-	expression tag	UNP A0A0D6FWC1
A	-1	SER	-	expression tag	UNP A0A0D6FWC1
A	0	HIS	-	expression tag	UNP A0A0D6FWC1
A	269	SER	-	linker	UNP A0A0D6FWC1
A	270	THR	-	linker	UNP A0A0D6FWC1
A	271	THR	-	linker	UNP A0A0D6FWC1
A	272	ARG	-	linker	UNP A0A0D6FWC1
A	273	PRO	-	linker	UNP A0A0D6FWC1
A	274	MET	-	linker	UNP A0A0D6FWC1
A	275	THR	-	linker	UNP A0A0D6FWC1
A	276	THR	-	linker	UNP A0A0D6FWC1
A	277	LEU	-	linker	UNP A0A0D6FWC1
A	671	LYS	-	expression tag	UNP A0A0F7J6T4
A	672	LEU	-	expression tag	UNP A0A0F7J6T4
A	673	ALA	-	expression tag	UNP A0A0F7J6T4
A	674	ALA	-	expression tag	UNP A0A0F7J6T4
A	675	ALA	-	expression tag	UNP A0A0F7J6T4
A	676	LEU	-	expression tag	UNP A0A0F7J6T4
A	677	GLU	-	expression tag	UNP A0A0F7J6T4
A	678	HIS	-	expression tag	UNP A0A0F7J6T4
A	679	HIS	-	expression tag	UNP A0A0F7J6T4
A	680	HIS	-	expression tag	UNP A0A0F7J6T4
A	681	HIS	-	expression tag	UNP A0A0F7J6T4
A	682	HIS	-	expression tag	UNP A0A0F7J6T4
A	683	HIS	-	expression tag	UNP A0A0F7J6T4
B	-298	SER	-	expression tag	UNP A0A0D6FWC1
B	-297	THR	-	expression tag	UNP A0A0D6FWC1
B	-296	THR	-	expression tag	UNP A0A0D6FWC1
B	-295	ARG	-	expression tag	UNP A0A0D6FWC1
B	-294	PRO	-	expression tag	UNP A0A0D6FWC1
B	-293	ALA	-	expression tag	UNP A0A0D6FWC1
B	-292	MET	-	expression tag	UNP A0A0D6FWC1
B	-291	GLY	-	expression tag	UNP A0A0D6FWC1
B	-290	SER	-	expression tag	UNP A0A0D6FWC1
B	-289	SER	-	expression tag	UNP A0A0D6FWC1
B	-288	HIS	-	expression tag	UNP A0A0D6FWC1
B	-287	HIS	-	expression tag	UNP A0A0D6FWC1
B	-286	HIS	-	expression tag	UNP A0A0D6FWC1
B	-285	HIS	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-284	HIS	-	expression tag	UNP A0A0D6FWC1
B	-283	HIS	-	expression tag	UNP A0A0D6FWC1
B	-282	SER	-	expression tag	UNP A0A0D6FWC1
B	-281	SER	-	expression tag	UNP A0A0D6FWC1
B	-280	GLY	-	expression tag	UNP A0A0D6FWC1
B	-279	LEU	-	expression tag	UNP A0A0D6FWC1
B	-278	VAL	-	expression tag	UNP A0A0D6FWC1
B	-277	PRO	-	expression tag	UNP A0A0D6FWC1
B	-276	ARG	-	expression tag	UNP A0A0D6FWC1
B	-275	GLY	-	expression tag	UNP A0A0D6FWC1
B	-274	SER	-	expression tag	UNP A0A0D6FWC1
B	-273	HIS	-	expression tag	UNP A0A0D6FWC1
B	-4	SER	-	linker	UNP A0A0D6FWC1
B	-3	THR	-	linker	UNP A0A0D6FWC1
B	-2	THR	-	linker	UNP A0A0D6FWC1
B	-1	ARG	-	linker	UNP A0A0D6FWC1
B	0	PRO	-	linker	UNP A0A0D6FWC1
B	1	MET	-	linker	UNP A0A0D6FWC1
B	2	THR	-	linker	UNP A0A0D6FWC1
B	3	THR	-	linker	UNP A0A0D6FWC1
B	4	LEU	-	linker	UNP A0A0D6FWC1
B	398	LYS	-	expression tag	UNP A0A0F7J6T4
B	399	LEU	-	expression tag	UNP A0A0F7J6T4
B	400	ALA	-	expression tag	UNP A0A0F7J6T4
B	401	ALA	-	expression tag	UNP A0A0F7J6T4
B	402	ALA	-	expression tag	UNP A0A0F7J6T4
B	403	LEU	-	expression tag	UNP A0A0F7J6T4
B	404	GLU	-	expression tag	UNP A0A0F7J6T4
B	405	HIS	-	expression tag	UNP A0A0F7J6T4
B	406	HIS	-	expression tag	UNP A0A0F7J6T4
B	407	HIS	-	expression tag	UNP A0A0F7J6T4
B	408	HIS	-	expression tag	UNP A0A0F7J6T4
B	409	HIS	-	expression tag	UNP A0A0F7J6T4
B	410	HIS	-	expression tag	UNP A0A0F7J6T4
C	-25	SER	-	expression tag	UNP A0A0D6FWC1
C	-24	THR	-	expression tag	UNP A0A0D6FWC1
C	-23	THR	-	expression tag	UNP A0A0D6FWC1
C	-22	ARG	-	expression tag	UNP A0A0D6FWC1
C	-21	PRO	-	expression tag	UNP A0A0D6FWC1
C	-20	ALA	-	expression tag	UNP A0A0D6FWC1
C	-19	MET	-	expression tag	UNP A0A0D6FWC1
C	-18	GLY	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP A0A0D6FWC1
C	-16	SER	-	expression tag	UNP A0A0D6FWC1
C	-15	HIS	-	expression tag	UNP A0A0D6FWC1
C	-14	HIS	-	expression tag	UNP A0A0D6FWC1
C	-13	HIS	-	expression tag	UNP A0A0D6FWC1
C	-12	HIS	-	expression tag	UNP A0A0D6FWC1
C	-11	HIS	-	expression tag	UNP A0A0D6FWC1
C	-10	HIS	-	expression tag	UNP A0A0D6FWC1
C	-9	SER	-	expression tag	UNP A0A0D6FWC1
C	-8	SER	-	expression tag	UNP A0A0D6FWC1
C	-7	GLY	-	expression tag	UNP A0A0D6FWC1
C	-6	LEU	-	expression tag	UNP A0A0D6FWC1
C	-5	VAL	-	expression tag	UNP A0A0D6FWC1
C	-4	PRO	-	expression tag	UNP A0A0D6FWC1
C	-3	ARG	-	expression tag	UNP A0A0D6FWC1
C	-2	GLY	-	expression tag	UNP A0A0D6FWC1
C	-1	SER	-	expression tag	UNP A0A0D6FWC1
C	0	HIS	-	expression tag	UNP A0A0D6FWC1
C	269	SER	-	linker	UNP A0A0D6FWC1
C	270	THR	-	linker	UNP A0A0D6FWC1
C	271	THR	-	linker	UNP A0A0D6FWC1
C	272	ARG	-	linker	UNP A0A0D6FWC1
C	273	PRO	-	linker	UNP A0A0D6FWC1
C	274	MET	-	linker	UNP A0A0D6FWC1
C	275	THR	-	linker	UNP A0A0D6FWC1
C	276	THR	-	linker	UNP A0A0D6FWC1
C	277	LEU	-	linker	UNP A0A0D6FWC1
C	671	LYS	-	expression tag	UNP A0A0F7J6T4
C	672	LEU	-	expression tag	UNP A0A0F7J6T4
C	673	ALA	-	expression tag	UNP A0A0F7J6T4
C	674	ALA	-	expression tag	UNP A0A0F7J6T4
C	675	ALA	-	expression tag	UNP A0A0F7J6T4
C	676	LEU	-	expression tag	UNP A0A0F7J6T4
C	677	GLU	-	expression tag	UNP A0A0F7J6T4
C	678	HIS	-	expression tag	UNP A0A0F7J6T4
C	679	HIS	-	expression tag	UNP A0A0F7J6T4
C	680	HIS	-	expression tag	UNP A0A0F7J6T4
C	681	HIS	-	expression tag	UNP A0A0F7J6T4
C	682	HIS	-	expression tag	UNP A0A0F7J6T4
C	683	HIS	-	expression tag	UNP A0A0F7J6T4
D	-298	SER	-	expression tag	UNP A0A0D6FWC1
D	-297	THR	-	expression tag	UNP A0A0D6FWC1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-296	THR	-	expression tag	UNP A0A0D6FWC1
D	-295	ARG	-	expression tag	UNP A0A0D6FWC1
D	-294	PRO	-	expression tag	UNP A0A0D6FWC1
D	-293	ALA	-	expression tag	UNP A0A0D6FWC1
D	-292	MET	-	expression tag	UNP A0A0D6FWC1
D	-291	GLY	-	expression tag	UNP A0A0D6FWC1
D	-290	SER	-	expression tag	UNP A0A0D6FWC1
D	-289	SER	-	expression tag	UNP A0A0D6FWC1
D	-288	HIS	-	expression tag	UNP A0A0D6FWC1
D	-287	HIS	-	expression tag	UNP A0A0D6FWC1
D	-286	HIS	-	expression tag	UNP A0A0D6FWC1
D	-285	HIS	-	expression tag	UNP A0A0D6FWC1
D	-284	HIS	-	expression tag	UNP A0A0D6FWC1
D	-283	HIS	-	expression tag	UNP A0A0D6FWC1
D	-282	SER	-	expression tag	UNP A0A0D6FWC1
D	-281	SER	-	expression tag	UNP A0A0D6FWC1
D	-280	GLY	-	expression tag	UNP A0A0D6FWC1
D	-279	LEU	-	expression tag	UNP A0A0D6FWC1
D	-278	VAL	-	expression tag	UNP A0A0D6FWC1
D	-277	PRO	-	expression tag	UNP A0A0D6FWC1
D	-276	ARG	-	expression tag	UNP A0A0D6FWC1
D	-275	GLY	-	expression tag	UNP A0A0D6FWC1
D	-274	SER	-	expression tag	UNP A0A0D6FWC1
D	-273	HIS	-	expression tag	UNP A0A0D6FWC1
D	-4	SER	-	linker	UNP A0A0D6FWC1
D	-3	THR	-	linker	UNP A0A0D6FWC1
D	-2	THR	-	linker	UNP A0A0D6FWC1
D	-1	ARG	-	linker	UNP A0A0D6FWC1
D	0	PRO	-	linker	UNP A0A0D6FWC1
D	1	MET	-	linker	UNP A0A0D6FWC1
D	2	THR	-	linker	UNP A0A0D6FWC1
D	3	THR	-	linker	UNP A0A0D6FWC1
D	4	LEU	-	linker	UNP A0A0D6FWC1
D	398	LYS	-	expression tag	UNP A0A0F7J6T4
D	399	LEU	-	expression tag	UNP A0A0F7J6T4
D	400	ALA	-	expression tag	UNP A0A0F7J6T4
D	401	ALA	-	expression tag	UNP A0A0F7J6T4
D	402	ALA	-	expression tag	UNP A0A0F7J6T4
D	403	LEU	-	expression tag	UNP A0A0F7J6T4
D	404	GLU	-	expression tag	UNP A0A0F7J6T4
D	405	HIS	-	expression tag	UNP A0A0F7J6T4
D	406	HIS	-	expression tag	UNP A0A0F7J6T4

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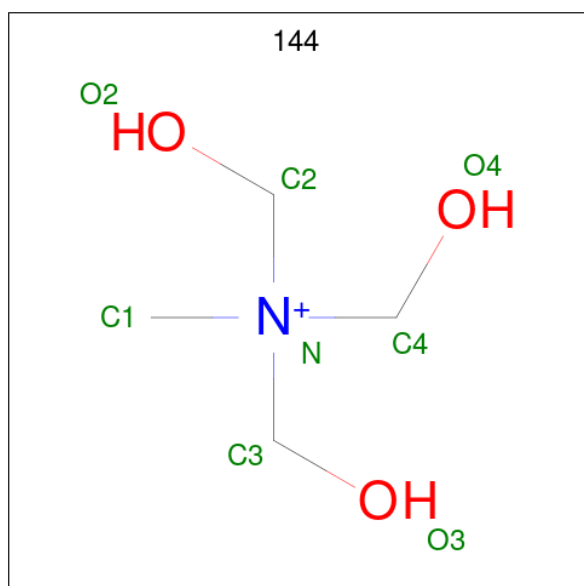
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Chain	Residue	Modelled	Actual	Comment	Reference
D	407	HIS	-	expression tag	UNP A0A0F7J6T4
D	408	HIS	-	expression tag	UNP A0A0F7J6T4
D	409	HIS	-	expression tag	UNP A0A0F7J6T4
D	410	HIS	-	expression tag	UNP A0A0F7J6T4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

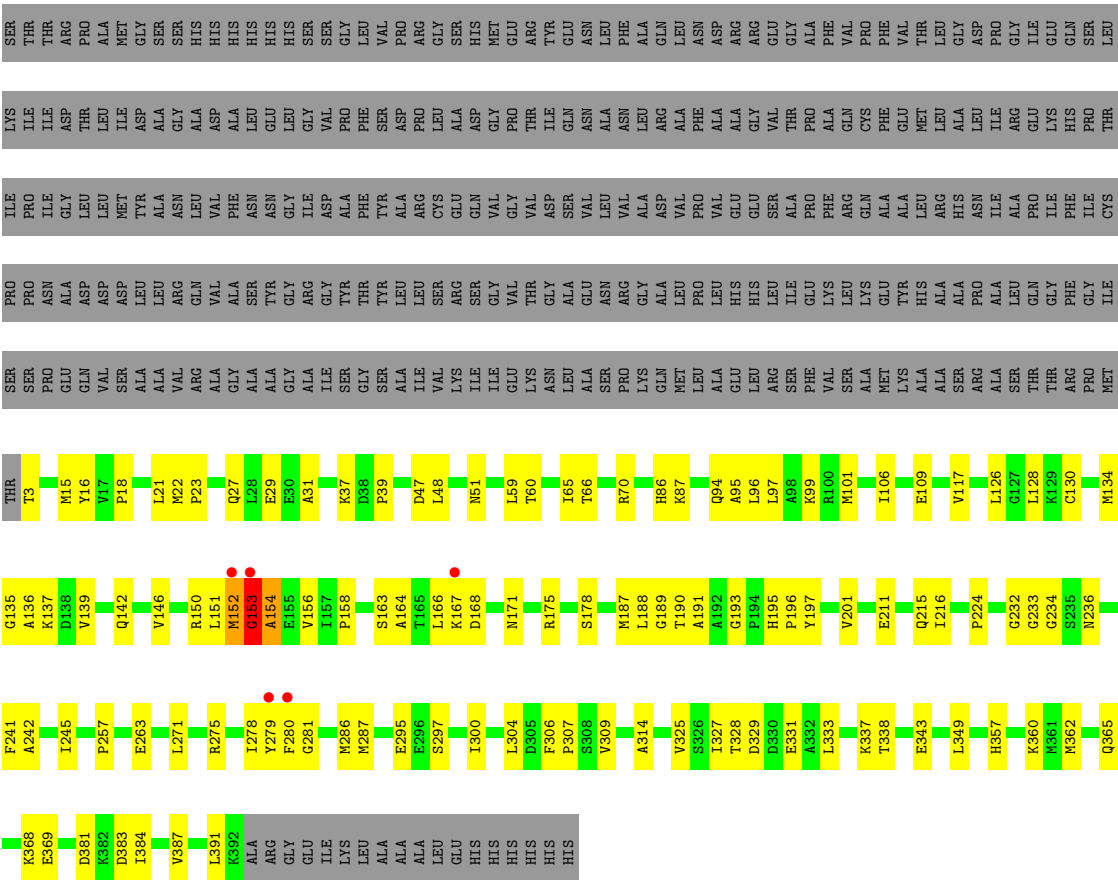
- Molecule 3 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (CCD ID: 144) (formula: C₄H₁₂NO₃) (labeled as "Ligand of Interest" by depositor).



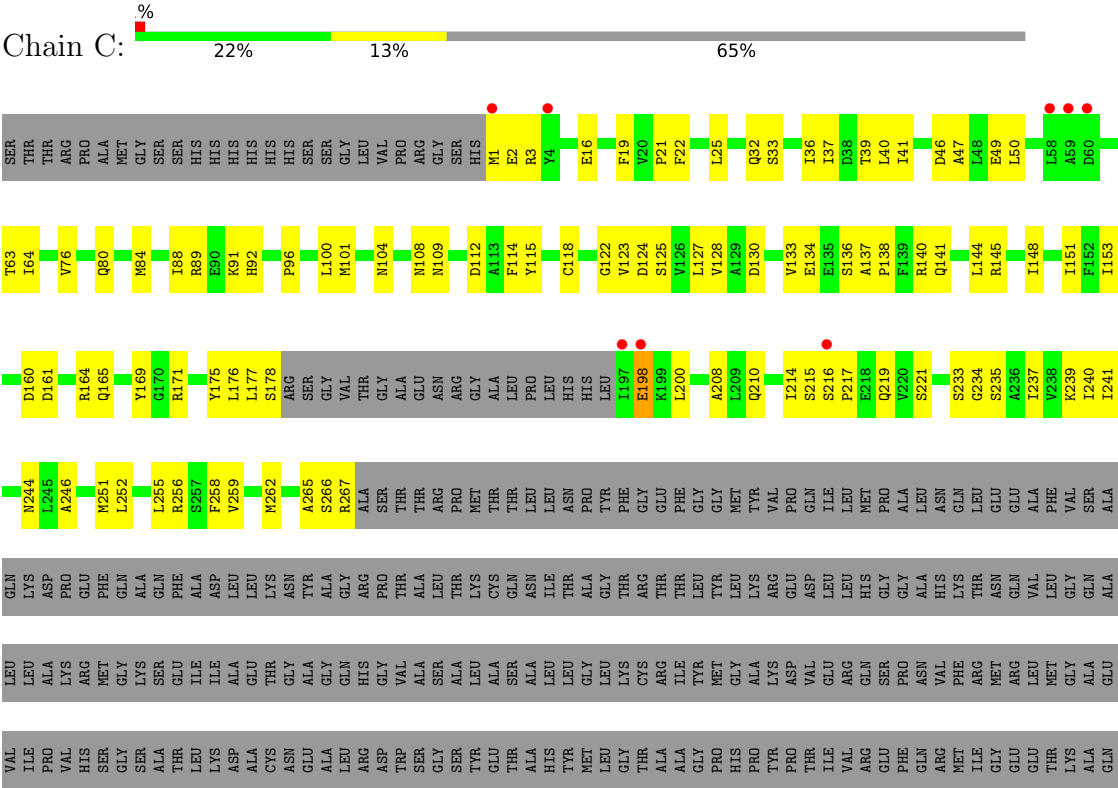
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O		0	0
			8	4	1	3			
3	D	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	15	Total 15	O 15	0	0
4	C	6	Total 6	O 6	0	0
4	D	14	Total 14	O 14	0	0

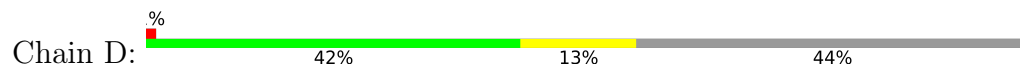


● Molecule 1: Tryptophan synthase alpha chain,Tryptophan synthase beta chain



[illegible]

- Molecule 1: Tryptophan synthase alpha chain, Tryptophan synthase beta chain



HIS	A294	L166	T2	SER	PRO	TLE	LYS	SER	THR
	P285	K167	T3		ASN				
HIS	M286	D168	P7	GLU	ALA	GLY	ASP	THR	ARG
	M287	S180	M15	GLN	ASP	LEU	LEU	THR	PRO
HIS	E296	T183	Y16	VAL	ASP	MET	ILE	LEU	ALA
	T300	M187	Y17	SER	ASP	TYR	ASP	ASP	GLY
HIS	L304	L188	M22	ALA	LEU	ALA	ALA	ALA	SER
	V309	G189	N51	VAL	GLN	ASN	GLY	ALA	HIS
HIS	G310	T190	Q63	ALA	VAL	VAL	ASP	ASP	HIS
	P311	G193	N64	GLY	ALA	PHE	ALA	ALA	HIS
HIS	Q312	P196	I65	ALA	SER	ASN	LEU	LEU	HIS
	L327	P196	I65	GLY	GLY	ASN	LEU	LEU	SER
HIS	E331	I200	T71	ALA	ARG	ILE	GLY	GLY	SER
	A332	V201	H86	ILE	GLY	ASP	VAL	VAL	SER
HIS	L333	R202	H86	SER	TYR	PHE	PRO	PRO	GLY
	L339	E210	V91	SER	TYR	TYR	ASP	ASP	VAL
HIS	G340	K213	Q94	ALA	LEU	ALA	ASP	ASP	PRO
	R341	K213	A95	ILE	LEU	ARG	PRO	PRO	ARG
HIS	P347	I216	L96	VAL	SER	CYS	LEU	LEU	GLY
	A348	I216	L96	LYS	ARG	GLN	ALA	ALA	SER
HIS	L355	R222	M101	ILE	LEU	VAL	GLY	GLY	HIS
	L359	R222	M101	VAL	LEU	GLY	VAL	VAL	ASN
HIS	P363	R223	A108	GLY	GLY	ASP	THR	THR	ARG
	L363	R223	E109	ASN	THR	ASP	ILE	ILE	TYR
HIS	Q370	P224	V117	GLN	GLY	GLY	THR	THR	ASN
	V373	D225	V117	ALA	ALA	VAL	ASN	ASN	ASN
HIS	G380	A237	L126	PRO	ARG	VAL	ASN	ASN	PHE
	P381	I238	G130	LYS	GLY	ALA	LEU	LEU	ALA
HIS	K382	D243	I132	GLN	ALA	ASP	ARG	ARG	GLN
	D383	D243	Y133	MET	LEU	VAL	GLY	GLY	GLY
HIS	L394	D247	G135	LEU	LEU	GLU	VAL	VAL	ASN
	L390	E256	V146	SER	LEU	ARG	GLN	GLN	VAL
HIS	G395	P257	M149	VAL	LYS	GLN	CYS	CYS	PHE
	GLU	H287	M149	MET	GLY	ALA	PHE	PHE	VAL
HIS	M289	G268	M152	LYS	TYR	ALA	GLU	GLU	VAL
	L270	A289	M152	ALA	HIS	LEU	MET	MET	LEU
HIS	ALA	P270	L271	ALA	ALA	HIS	ALA	ALA	GLY
	ALA	L271	P158	SER	ALA	HIS	ALA	ALA	ASP
HIS	ALA	I278	V159	ARG	PRO	ASN	LEU	LEU	PRO
	ALA	I278	H160	ALA	ALA	ILE	ILE	ILE	ASN
HIS	LEU	Y279	S161	SER	LEU	ALA	ARG	ARG	GLY
	GLU	F280	G162	THR	GLN	PRO	GLU	GLU	ILE
HIS	HIS	G281	S163	THR	GLY	ILE	LYS	LYS	GLN
	HIS	M282	A164	ARG	PHE	PHE	THR	THR	SER
HIS	P283	T165	T165	PRO	GLY	ILE	PRO	PRO	THR
	P283	T165	T165	MET	THR	CYS	THR	THR	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.37Å 95.97Å 184.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 2.50 47.10 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.10-2.50) 99.7 (47.10-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.190 , 0.250 0.197 , 0.255	Depositor DCC
R_{free} test set	2911 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9806	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: NA, 144

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	0.41	0/1958	0.60	0/2663
1	B	0.43	0/3012	0.64	4/4069 (0.1%)
1	C	0.36	0/1912	0.55	0/2598
1	D	0.45	1/3040 (0.0%)	0.62	0/4108
All	All	0.42	1/9922 (0.0%)	0.61	4/13438 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	101	MET	CA-C	7.17	1.62	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	MET	CB-CG-SD	-7.16	91.21	112.70
1	B	152	MET	CA-C-N	5.32	131.83	121.41
1	B	152	MET	C-N-CA	5.32	131.83	121.41
1	B	153	GLY	N-CA-C	5.25	125.62	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	153	GLY	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	1919	0	1928	81	0
1	B	2954	0	2931	104	2
1	C	1876	0	1869	94	0
1	D	2982	0	2944	84	2
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	B	8	0	12	14	0
3	D	8	12	12	10	0
4	A	10	0	0	2	0
4	B	15	0	0	2	0
4	C	6	0	0	5	0
4	D	14	0	0	2	0
All	All	9794	12	9696	371	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (371) 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)
3:B:502:144:N	3:B:502:144:C2	1.77	1.46
3:D:502:144:N	3:D:502:144:C2	1.86	1.37
1:B:137:LYS:HB2	1:B:164:ALA:HB3	1.33	1.08
1:C:140:ARG:HD3	1:C:169:TYR:HB3	1.42	1.00
1:C:40:LEU:HD23	1:C:259:VAL:HG21	1.49	0.95
1:D:134:MET:HE1	1:D:146:VAL:HG22	1.50	0.94
1:D:282:MET:HE2	1:D:284:ALA:HB2	1.52	0.92
3:B:502:144:C2	3:B:502:144:C1	2.49	0.90
1:C:22:PHE:HE2	1:C:64:ILE:HD13	1.37	0.90
1:D:15:MET:HB3	1:D:22:MET:HE1	1.53	0.90
1:C:176:LEU:HD23	1:C:208:ALA:HB1	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:OD1	1:B:275:ARG:NH2	2.06	0.88
1:B:106:ILE:HD11	1:B:128:LEU:HD13	1.54	0.87
1:C:160:ASP:OD1	1:C:164:ARG:NH1	2.08	0.86
1:B:234:GLY:H	3:B:502:144:H21	1.40	0.86
1:D:282:MET:HE1	1:D:311:PRO:HD3	1.57	0.83
1:B:137:LYS:H	1:B:164:ALA:CB	1.90	0.83
1:C:33:SER:OG	4:C:701:HOH:O	1.97	0.83
1:D:395:GLY:O	4:D:601:HOH:O	1.97	0.82
1:B:163:SER:OG	1:B:168:ASP:OD2	1.98	0.82
3:D:502:144:C2	3:D:502:144:C4	2.56	0.82
1:B:137:LYS:H	1:B:164:ALA:HB1	1.45	0.82
1:D:282:MET:CE	1:D:311:PRO:HD3	2.11	0.81
1:A:7:LEU:CD1	1:A:11:LEU:HD11	2.11	0.80
1:B:150:ARG:HA	1:B:153:GLY:HA2	1.63	0.80
1:C:118:CYS:HB2	1:C:148:ILE:CD1	2.13	0.78
1:A:7:LEU:O	1:A:11:LEU:HD12	1.83	0.78
1:A:48:LEU:HD22	1:A:95:ILE:HD13	1.65	0.78
3:B:502:144:C2	3:B:502:144:C3	2.61	0.78
1:C:216:SER:O	1:C:262:MET:HE1	1.84	0.77
1:C:22:PHE:CE2	1:C:64:ILE:HD13	2.19	0.77
1:C:171:ARG:HG2	1:C:171:ARG:HH11	1.48	0.77
1:D:271:LEU:HG	1:D:309:VAL:HG11	1.67	0.77
1:B:328:THR:OG1	1:B:331:GLU:HG3	1.84	0.76
3:B:502:144:C2	3:B:502:144:C4	2.65	0.75
1:B:87:LYS:HE3	1:B:189:GLY:O	1.88	0.74
1:B:106:ILE:HD11	1:B:128:LEU:CD1	2.17	0.74
1:D:257:PRO:HG3	1:D:304:LEU:HB3	1.71	0.73
3:B:502:144:C1	3:B:502:144:O2	2.37	0.72
3:D:502:144:C2	3:D:502:144:C3	2.67	0.72
1:A:217:PRO:HB3	1:A:265:ALA:HB2	1.72	0.71
1:B:70:ARG:O	4:B:601:HOH:O	2.07	0.71
1:A:1:MET:HG2	1:A:2:GLU:OE2	1.91	0.71
3:D:502:144:O2	3:D:502:144:H42	1.91	0.70
1:B:3:THR:N	4:B:602:HOH:O	2.24	0.70
1:C:112:ASP:OD2	1:C:145:ARG:NH2	2.20	0.69
1:B:300:ILE:HG23	1:B:329:ASP:OD2	1.92	0.69
1:C:22:PHE:CD1	1:C:49:GLU:HG2	2.27	0.69
1:C:153:ILE:HG23	1:C:177:LEU:HD13	1.73	0.68
1:C:176:LEU:CD2	1:C:208:ALA:HB1	2.23	0.68
1:C:214:ILE:O	1:C:233:SER:HB2	1.93	0.68
1:B:146:VAL:HG13	1:B:156:VAL:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:TYR:OH	4:C:702:HOH:O	2.10	0.67
1:B:106:ILE:HD12	1:B:128:LEU:HB3	1.76	0.67
1:C:84:MET:O	1:C:88:ILE:HG13	1.94	0.67
1:C:164:ARG:HG2	1:C:164:ARG:HH11	1.60	0.67
1:C:169:TYR:O	4:C:703:HOH:O	2.12	0.67
1:C:171:ARG:HG2	1:C:171:ARG:NH1	2.09	0.66
1:B:232:GLY:H	3:B:502:144:H22	1.60	0.66
1:C:32:GLN:O	1:C:36:ILE:HG13	1.95	0.66
1:D:3:THR:HG21	1:D:7:PRO:HG3	1.78	0.66
1:D:134:MET:O	1:D:158:PRO:HA	1.96	0.66
1:C:217:PRO:N	1:C:262:MET:HE3	2.10	0.66
1:A:214:ILE:O	1:A:233:SER:HB2	1.94	0.66
1:B:117:VAL:HG13	1:B:152:MET:HE1	1.78	0.66
1:D:65:ILE:HD12	1:D:359:LEU:HD21	1.79	0.65
1:A:7:LEU:HG	1:A:11:LEU:CD1	2.27	0.65
1:B:233:GLY:N	3:B:502:144:H21	2.11	0.65
1:C:22:PHE:HD1	1:C:49:GLU:HG2	1.59	0.65
1:A:23:VAL:HG21	1:A:37:ILE:CD1	2.26	0.65
1:C:221:SER:OG	1:C:265:ALA:O	2.14	0.65
1:D:15:MET:CB	1:D:22:MET:HE1	2.26	0.65
1:D:222[A]:ARG:HH22	1:D:225:ASP:CG	2.06	0.64
1:A:11:LEU:HD22	1:A:18:ALA:HB2	1.78	0.64
1:B:130:CYS:O	1:B:154:ALA:HB1	1.98	0.64
1:C:63:THR:HG21	1:C:239:LYS:HD2	1.79	0.64
1:C:118:CYS:HB2	1:C:148:ILE:HD11	1.80	0.63
1:A:22:PHE:HB3	1:A:234:GLY:HA2	1.81	0.63
1:B:216:ILE:HG21	1:B:224:PRO:HD3	1.80	0.62
3:D:502:144:C2	3:D:502:144:C1	2.77	0.62
1:C:141:GLN:HB3	1:C:145:ARG:NH1	2.14	0.62
1:A:141:GLN:HG2	1:A:145:ARG:HH12	1.64	0.62
1:D:188:LEU:HD23	1:D:189:GLY:N	2.15	0.61
1:C:216:SER:O	1:C:262:MET:CE	2.48	0.61
1:C:91:LYS:HG2	1:C:92:HIS:CD2	2.36	0.61
1:A:23:VAL:HG21	1:A:37:ILE:HD11	1.82	0.61
1:A:40:LEU:HD23	1:A:259:VAL:HG21	1.81	0.61
1:C:215:SER:N	1:C:219:GLN:OE1	2.34	0.61
1:C:36:ILE:HG23	1:C:255:LEU:CD1	2.31	0.61
1:B:16:TYR:O	1:B:281:GLY:HA2	2.01	0.61
1:B:188:LEU:HD23	1:B:190:THR:H	1.66	0.60
1:A:7:LEU:HD11	1:A:11:LEU:HD11	1.81	0.60
1:B:106:ILE:HD12	1:B:128:LEU:CB	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:C	1:B:153:GLY:H	2.09	0.60
1:B:134:MET:O	1:B:158:PRO:HA	2.02	0.60
1:A:141:GLN:HG2	1:A:145:ARG:NH1	2.17	0.60
1:C:1:MET:HE2	1:C:2:GLU:OE1	2.02	0.60
1:D:300:ILE:HD11	1:D:390:ILE:CD1	2.31	0.60
1:B:327:ILE:HG23	1:B:331:GLU:HB2	1.83	0.59
1:C:216:SER:C	1:C:262:MET:HE3	2.27	0.59
1:A:192:PRO:HB2	1:A:194:HIS:ND1	2.17	0.59
1:B:151:LEU:C	1:B:153:GLY:H	2.09	0.59
1:B:137:LYS:HB2	1:B:164:ALA:CB	2.22	0.59
1:A:151:ILE:HA	4:A:708:HOH:O	2.02	0.59
1:D:210:GLU:HG2	1:D:243:ASP:OD2	2.03	0.58
1:A:21:PRO:HB3	1:A:237:ILE:HD13	1.84	0.58
1:A:69:LEU:HD11	1:C:246:ALA:HA	1.85	0.58
1:A:33:SER:O	1:A:37:ILE:HG12	2.04	0.58
1:A:7:LEU:O	1:A:11:LEU:CD1	2.50	0.58
1:A:130:ASP:OD1	1:A:130:ASP:N	2.37	0.58
1:A:21:PRO:HB3	1:A:237:ILE:CD1	2.32	0.57
1:A:140:ARG:HD3	1:A:169:TYR:HB3	1.86	0.57
1:A:194:HIS:O	1:A:198:GLU:HG2	2.04	0.57
1:C:125:SER:HB2	1:C:151:ILE:HD11	1.86	0.57
1:C:169:TYR:HA	4:C:703:HOH:O	2.03	0.57
1:B:150:ARG:CA	1:B:153:GLY:HA2	2.34	0.57
1:C:96:PRO:HA	1:C:124:ASP:OD2	2.03	0.57
1:C:21:PRO:HD2	1:C:47:ALA:O	2.05	0.57
1:A:84:MET:O	1:A:88:ILE:HG13	2.04	0.57
1:B:47:ASP:OD1	1:B:51:ASN:ND2	2.37	0.57
1:C:216:SER:C	1:C:262:MET:CE	2.77	0.57
1:A:21:PRO:CB	1:A:237:ILE:HD13	2.34	0.57
1:D:86:HIS:HE1	3:D:502:144:H32	1.70	0.56
1:D:180:SER:O	1:D:183:THR:HG22	2.05	0.56
1:A:199:LYS:NZ	1:A:203:TYR:OH	2.38	0.56
1:B:234:GLY:H	3:B:502:144:C2	2.15	0.56
1:C:244:ASN:HB2	1:C:251:MET:HB2	1.87	0.56
1:D:163:SER:HB2	1:D:168:ASP:OD2	2.04	0.56
1:C:22:PHE:HB3	1:C:234:GLY:HA2	1.86	0.56
1:D:95:ALA:CB	1:D:126:LEU:HD12	2.36	0.56
3:D:502:144:C2	3:D:502:144:H42	2.32	0.56
1:B:142:GLN:O	1:B:146:VAL:HG23	2.05	0.56
1:B:150:ARG:O	1:B:153:GLY:CA	2.54	0.56
1:D:202:ARG:NH1	1:D:312:GLN:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:HA	1:A:32:GLN:NE2	2.21	0.56
1:B:135:GLY:HA3	1:B:164:ALA:O	2.06	0.56
1:D:95:ALA:HB1	1:D:126:LEU:HD12	1.88	0.56
1:C:134:GLU:OE1	1:C:134:GLU:N	2.36	0.56
1:D:86:HIS:CE1	1:D:236:ASN:HB3	2.41	0.55
1:D:300:ILE:HD11	1:D:390:ILE:HD11	1.86	0.55
1:B:166:LEU:CD2	1:B:167:LYS:HE2	2.36	0.55
1:A:197:ILE:HG22	1:A:201:LYS:HE2	1.88	0.55
1:B:86:HIS:CE1	1:B:236:ASN:HB3	2.41	0.55
1:A:263:LYS:HD2	1:A:263:LYS:O	2.07	0.55
1:B:136:ALA:N	1:B:164:ALA:HB1	2.22	0.55
1:C:153:ILE:CG2	1:C:177:LEU:HD13	2.36	0.55
1:A:113:ALA:O	1:A:117:ARG:HG3	2.07	0.54
1:B:175:ARG:O	1:B:178:SER:HB2	2.07	0.54
1:D:135:GLY:HA2	1:D:159:VAL:HG22	1.88	0.54
1:B:109:GLU:OE1	1:B:109:GLU:N	2.37	0.54
1:C:39:THR:HG23	1:C:256:ARG:HG3	1.87	0.54
1:D:2:THR:O	1:D:3:THR:OG1	2.22	0.54
1:A:49:GLU:HA	1:A:98:GLY:O	2.08	0.54
1:D:327:ILE:HG23	1:D:331:GLU:HB2	1.89	0.54
1:B:106:ILE:CD1	1:B:128:LEU:CB	2.86	0.54
1:C:37:ILE:HG21	1:C:88:ILE:HD13	1.89	0.54
1:D:163:SER:HB2	1:D:168:ASP:CG	2.32	0.53
1:A:170:GLY:O	1:A:171:ARG:HD3	2.09	0.53
1:D:339:LEU:HD13	1:D:355:LEU:CD2	2.39	0.53
1:C:40:LEU:HD23	1:C:259:VAL:CG2	2.29	0.53
1:B:97:LEU:O	1:B:101:MET:HG3	2.09	0.53
1:B:59:LEU:HB2	1:B:215:GLN:OE1	2.10	0.52
1:A:11:LEU:CD2	1:A:18:ALA:HB2	2.39	0.52
1:A:127:LEU:C	1:A:127:LEU:HD23	2.35	0.52
1:B:211:GLU:O	1:B:215:GLN:HG3	2.09	0.52
1:C:25:LEU:HG	1:C:50:LEU:HB3	1.92	0.52
1:C:141:GLN:HB3	1:C:145:ARG:HH12	1.72	0.52
1:C:178:SER:HB2	1:C:210:GLN:HE22	1.75	0.52
1:C:91:LYS:HB3	1:C:92:HIS:HD2	1.73	0.52
1:A:112:ASP:OD2	1:A:145:ARG:NH2	2.40	0.52
1:D:282:MET:HE1	1:D:311:PRO:CD	2.37	0.52
1:A:6:ASN:O	1:A:10:GLN:HG2	2.09	0.52
1:D:216:ILE:HG21	1:D:224:PRO:HD3	1.92	0.52
1:A:62:PRO:O	1:A:66:ASN:ND2	2.40	0.51
1:D:196:PRO:O	1:D:200:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ILE:HD12	1:C:92:HIS:CE1	2.45	0.51
1:A:59:ALA:HB2	1:B:18:PRO:HG3	1.93	0.51
1:A:7:LEU:HG	1:A:11:LEU:HD13	1.93	0.51
1:C:76:VAL:HA	1:C:80:GLN:OE1	2.11	0.51
1:D:202:ARG:HG3	1:D:238:ILE:HG13	1.93	0.51
1:A:244:ASN:HB2	1:A:251:MET:HB2	1.92	0.51
1:B:331:GLU:OE2	1:B:360:LYS:NZ	2.44	0.51
1:D:123:SER:OG	1:D:130:CYS:HB2	2.11	0.51
1:D:341:ARG:HA	1:D:341:ARG:NE	2.26	0.51
1:B:234:GLY:N	3:B:502:144:H21	2.20	0.50
3:B:502:144:C2	3:B:502:144:H31	2.41	0.50
1:D:347:PRO:O	1:D:380:GLY:HA3	2.10	0.50
1:A:258:PHE:CZ	1:A:262:MET:HE2	2.47	0.50
1:D:193:GLY:HA2	1:D:280:PHE:O	2.11	0.50
1:A:10:GLN:HB2	1:A:14:ARG:NH2	2.27	0.50
1:A:247:SER:HB3	1:D:296:GLU:OE2	2.11	0.50
1:A:40:LEU:CD2	1:A:259:VAL:HG21	2.41	0.50
1:D:339:LEU:HD13	1:D:355:LEU:HD21	1.94	0.50
1:D:94:GLN:CB	1:D:187:MET:HE2	2.42	0.50
1:D:91:VAL:HG12	1:D:122:ALA:HB2	1.93	0.50
1:C:153:ILE:HA	1:C:175:TYR:O	2.11	0.50
1:D:163:SER:O	1:D:164:ALA:HB3	2.12	0.49
1:B:383:ASP:O	1:B:387:VAL:HG23	2.11	0.49
1:A:7:LEU:CG	1:A:11:LEU:HD11	2.43	0.49
1:D:227:VAL:HG12	1:D:373:VAL:HB	1.95	0.49
1:D:359:LEU:O	1:D:363:ARG:HG3	2.13	0.49
1:B:257:PRO:HG3	1:B:304:LEU:HB3	1.94	0.49
1:D:382:LYS:HE3	1:D:383:ASP:OD2	2.12	0.48
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.94	0.48
1:B:94:GLN:HB3	1:B:187:MET:HE2	1.95	0.48
1:B:271:LEU:HD23	1:B:271:LEU:HA	1.52	0.48
1:B:23:PRO:O	1:B:27:GLN:HG3	2.13	0.48
1:B:139:VAL:HG21	1:B:158:PRO:HB3	1.95	0.48
1:B:306:PHE:CD1	1:B:307:PRO:HD2	2.47	0.48
1:A:244:ASN:CB	1:A:251:MET:HB2	2.44	0.48
1:C:101:MET:HE2	1:C:114:PHE:CE1	2.48	0.48
1:C:3:ARG:HD2	1:C:124:ASP:OD2	2.14	0.48
1:C:1:MET:HB3	1:C:2:GLU:OE1	2.13	0.48
1:A:7:LEU:HG	1:A:11:LEU:HD11	1.95	0.48
1:A:86:ALA:HB2	1:A:121:VAL:CG2	2.43	0.48
1:B:300:ILE:HD12	1:B:333:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HD3	1:C:169:TYR:CB	2.29	0.47
1:A:48:LEU:CD2	1:A:95:ILE:HD13	2.42	0.47
1:D:108:ALA:O	1:D:132:ILE:HA	2.13	0.47
1:D:188:LEU:HD23	1:D:190:THR:H	1.79	0.47
1:D:282:MET:HE3	1:D:311:PRO:HD3	1.91	0.47
1:B:263:GLU:H	1:B:263:GLU:CD	2.22	0.47
1:C:101:MET:HE2	1:C:114:PHE:CZ	2.49	0.47
1:C:198[A]:GLU:HG2	1:C:200:LEU:H	1.79	0.47
1:B:137:LYS:H	1:B:164:ALA:HB3	1.77	0.47
1:B:166:LEU:HD22	1:B:167:LYS:HE2	1.97	0.47
1:A:96:PRO:HA	1:A:124:ASP:OD2	2.15	0.47
1:B:3:THR:HB	1:B:29:GLU:OE2	2.12	0.47
1:C:36:ILE:HD13	1:C:241:ILE:HD13	1.97	0.47
1:B:271:LEU:HD21	1:B:314:ALA:HA	1.97	0.47
1:C:267:ARG:CB	1:C:267:ARG:HH11	2.28	0.47
1:D:279:TYR:CG	1:D:280:PHE:N	2.83	0.47
1:A:197:ILE:O	1:A:201:LYS:HG3	2.14	0.47
1:C:19:PHE:N	1:C:46:ASP:OD2	2.37	0.47
1:C:140:ARG:O	1:C:144:LEU:HG	2.14	0.47
1:A:164:ARG:NE	4:A:701:HOH:O	2.26	0.47
1:A:25:LEU:HG	1:A:50:LEU:HB3	1.98	0.46
1:B:190:THR:OG1	1:B:191:ALA:N	2.49	0.46
1:D:123:SER:CB	1:D:130:CYS:HB2	2.44	0.46
1:D:300:ILE:CD1	1:D:390:ILE:HD11	2.45	0.46
1:B:241:PHE:O	1:B:242:ALA:C	2.58	0.46
3:B:502:144:O2	3:B:502:144:H13	2.15	0.46
1:A:80:GLN:O	1:A:84:MET:HG3	2.15	0.46
1:B:37:LYS:O	1:B:39:PRO:HD3	2.14	0.46
1:B:300:ILE:CD1	1:B:333:LEU:CD2	2.93	0.46
1:B:381:ASP:O	1:B:384:ILE:HG13	2.16	0.46
1:B:96:LEU:HD23	1:B:96:LEU:HA	1.79	0.46
1:B:197:TYR:O	1:B:201:VAL:HG23	2.16	0.46
1:B:232:GLY:H	3:B:502:144:C2	2.26	0.46
1:C:100:LEU:CD1	1:C:127:LEU:HD13	2.46	0.46
1:C:164:ARG:HH11	1:C:164:ARG:CG	2.25	0.46
1:C:176:LEU:HD23	1:C:208:ALA:CB	2.37	0.46
1:B:279:TYR:HB3	1:B:286:MET:HE1	1.98	0.46
1:A:164:ARG:HD2	1:A:203:TYR:CD2	2.50	0.45
1:D:117:VAL:HG13	1:D:152:MET:HE1	1.98	0.45
1:A:58:LEU:C	1:A:60:ASP:H	2.24	0.45
1:A:100:LEU:C	1:A:100:LEU:HD23	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLY:HA3	1:B:164:ALA:C	2.41	0.45
1:B:195:HIS:ND1	1:B:196:PRO:HA	2.31	0.45
1:D:300:ILE:CD1	1:D:390:ILE:CD1	2.94	0.45
1:C:91:LYS:HG2	1:C:92:HIS:NE2	2.32	0.45
1:D:109:GLU:N	1:D:109:GLU:OE1	2.50	0.45
1:D:213:LYS:NZ	1:D:243:ASP:HB3	2.31	0.45
1:A:221:SER:HB3	1:A:265:ALA:O	2.16	0.45
1:C:130:ASP:OD1	1:C:130:ASP:N	2.41	0.45
1:D:94:GLN:HB3	1:D:187:MET:HE2	1.99	0.45
1:D:286:MET:HE2	1:D:286:MET:HB3	1.84	0.45
1:C:127:LEU:HD23	1:C:128:VAL:N	2.31	0.44
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.82	0.44
1:D:300:ILE:HD13	1:D:333:LEU:HD21	1.99	0.44
1:D:348:ALA:HA	1:D:380:GLY:HA2	1.98	0.44
1:B:325:VAL:HG21	1:B:357:HIS:CE1	2.53	0.44
1:C:235:SER:O	1:C:239:LYS:HB2	2.18	0.44
1:C:237:ILE:HD13	1:C:258:PHE:HD2	1.82	0.44
1:D:17:VAL:HG22	1:D:22:MET:CE	2.47	0.44
1:B:106:ILE:CD1	1:B:128:LEU:HB2	2.47	0.44
1:C:89:ARG:HG2	1:C:122:GLY:HA3	1.99	0.44
1:C:36:ILE:HG23	1:C:255:LEU:HD13	1.97	0.44
1:C:91:LYS:HB3	1:C:92:HIS:CD2	2.53	0.44
1:D:210:GLU:HG3	1:D:243:ASP:CG	2.43	0.44
1:D:300:ILE:CD1	1:D:333:LEU:HD21	2.47	0.44
1:A:214:ILE:O	1:A:233:SER:CB	2.65	0.44
1:D:267:HIS:CE1	1:D:287:MET:HE3	2.53	0.43
1:D:279:TYR:HB3	1:D:286:MET:HE1	1.99	0.43
1:A:23:VAL:HG11	1:A:40:LEU:HD11	2.00	0.43
1:D:268:GLY:O	1:D:270:PRO:HD2	2.19	0.43
1:C:104:ASN:HB2	1:D:278:ILE:O	2.19	0.43
1:B:65:ILE:HG12	1:B:343:GLU:HG2	1.99	0.43
1:D:132:ILE:HD13	1:D:149:MET:SD	2.59	0.43
1:D:190:THR:OG1	1:D:233:GLY:HA3	2.19	0.43
1:B:70:ARG:NH2	1:B:369:GLU:HB2	2.33	0.43
1:B:99:LYS:HG2	1:B:128:LEU:HD21	2.01	0.43
1:B:242:ALA:O	1:B:245:ILE:HG13	2.19	0.43
1:B:286:MET:HE2	1:B:286:MET:HB3	1.72	0.43
1:C:133:VAL:HG22	1:C:134:GLU:OE1	2.18	0.43
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.48	0.43
1:B:151:LEU:C	1:B:153:GLY:N	2.75	0.43
1:B:95:ALA:HB1	1:B:126:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:MET:HG3	1:B:195:HIS:HB3	2.00	0.43
1:B:365:GLN:HB3	1:B:368:LYS:HB2	2.00	0.43
1:C:63:THR:CG2	1:C:239:LYS:HD2	2.47	0.42
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.78	0.42
1:D:71:THR:HA	1:D:370:GLN:O	2.19	0.42
1:C:169:TYR:CA	4:C:703:HOH:O	2.65	0.42
1:C:217:PRO:CD	1:C:262:MET:HE3	2.48	0.42
1:D:163:SER:CB	1:D:168:ASP:CG	2.92	0.42
1:D:256:GLU:CD	1:D:271:LEU:HB2	2.43	0.42
1:A:111:ILE:HD12	1:A:138:PRO:HB2	2.02	0.42
1:D:160:HIS:O	1:D:162:GLY:N	2.53	0.42
1:D:279:TYR:O	1:D:282:MET:HG2	2.18	0.42
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.82	0.42
1:A:244:ASN:HD22	1:A:251:MET:HA	1.84	0.42
1:B:66:THR:HG22	1:B:362:MET:SD	2.60	0.42
1:A:214:ILE:HB	1:A:232:ILE:O	2.19	0.42
1:A:256:ARG:HE	1:A:256:ARG:HB2	1.67	0.42
1:A:36:ILE:HD13	1:A:241:ILE:HD13	2.01	0.42
1:B:171:ASN:HD22	1:B:171:ASN:C	2.26	0.42
1:C:240:ILE:HG21	1:C:255:LEU:HD23	2.01	0.42
1:D:96:LEU:HD23	1:D:96:LEU:HA	1.71	0.42
1:B:65:ILE:HG12	1:B:343:GLU:CG	2.50	0.42
1:C:22:PHE:HD1	1:C:49:GLU:O	2.02	0.42
1:D:341:ARG:NE	1:D:341:ARG:CA	2.83	0.42
1:A:199:LYS:HD2	1:A:202:GLU:OE1	2.20	0.42
1:D:94:GLN:HB2	1:D:187:MET:HE2	2.02	0.42
1:A:69:LEU:HD11	1:C:246:ALA:CA	2.49	0.41
3:B:502:144:H22	3:B:502:144:H31	2.02	0.41
1:C:136:SER:O	1:C:137:ALA:C	2.63	0.41
1:A:104:ASN:HB2	1:B:278:ILE:O	2.19	0.41
1:A:158:ALA:HB1	1:A:162:LEU:HD23	2.02	0.41
1:B:271:LEU:HG	1:B:309:VAL:HG11	2.01	0.41
1:D:282:MET:CE	1:D:311:PRO:CD	2.91	0.41
1:B:167:LYS:HA	1:B:167:LYS:HD3	1.76	0.41
1:B:391:LEU:N	1:B:391:LEU:CD1	2.83	0.41
1:D:232:GLY:HA3	3:D:502:144:H12	2.02	0.41
1:C:118:CYS:HB3	1:C:123:VAL:HB	2.02	0.41
1:B:65:ILE:HD12	1:B:338:THR:HG22	2.03	0.41
1:B:163:SER:O	1:B:168:ASP:OD2	2.39	0.41
1:B:166:LEU:C	1:B:166:LEU:HD23	2.46	0.41
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASP:O	1:C:165:GLN:HG3	2.20	0.41
1:C:108:ASN:ND2	1:C:109:ASN:OD1	2.54	0.41
1:D:300:ILE:HD11	1:D:390:ILE:HD12	2.01	0.41
1:B:193:GLY:HA2	1:B:280:PHE:O	2.21	0.41
1:B:287:MET:HB3	1:B:295:GLU:HG2	2.02	0.41
1:C:16:GLU:HB2	1:C:266:SER:O	2.20	0.41
1:C:40:LEU:CD2	1:C:259:VAL:HG21	2.35	0.41
1:B:22:MET:N	1:B:23:PRO:CD	2.84	0.41
1:B:337:LYS:HE3	1:B:337:LYS:HB2	1.62	0.41
1:C:41:ILE:HG21	1:C:92:HIS:ND1	2.36	0.41
1:C:198[A]:GLU:CD	1:C:198[A]:GLU:C	2.89	0.41
1:A:134:GLU:OE1	1:A:134:GLU:N	2.40	0.41
1:B:95:ALA:CB	1:B:126:LEU:HD12	2.50	0.41
1:C:123:VAL:HG12	1:C:124:ASP:N	2.36	0.41
1:C:137:ALA:HB3	1:C:138:PRO:HD3	2.02	0.41
1:D:17:VAL:CG2	1:D:22:MET:HE2	2.51	0.41
1:D:86:HIS:CE1	3:D:502:144:H32	2.55	0.41
1:D:256:GLU:OE2	1:D:271:LEU:HB2	2.21	0.41
1:A:21:PRO:CB	1:A:237:ILE:CD1	2.98	0.41
1:C:100:LEU:HD12	1:C:127:LEU:HB3	2.03	0.41
1:A:116:ALA:HB2	1:A:146:HIS:NE2	2.36	0.40
1:A:127:LEU:HD23	1:A:128:VAL:N	2.36	0.40
1:B:328:THR:HG1	1:B:331:GLU:HG3	1.85	0.40
1:D:363:ARG:NH2	4:D:602:HOH:O	2.34	0.40
1:B:287:MET:HE1	1:B:297:SER:HA	2.02	0.40
1:A:163:LEU:HD22	1:A:200:LEU:HG	2.01	0.40
1:B:70:ARG:HH21	1:B:369:GLU:HB2	1.86	0.40
1:A:153:ILE:HA	1:A:175:TYR:O	2.22	0.40
1:B:21:LEU:HD23	1:B:21:LEU:HA	1.83	0.40
1:D:384:ILE:HD12	1:D:384:ILE:HG23	1.75	0.40
1:B:31:ALA:HB2	1:B:101:MET:HE3	2.04	0.40
3:D:502:144:C2	3:D:502:144:H31	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:THR:OG1	1:D:51:ASN:O[3_544]	2.07	0.13
1:B:153:GLY:O	1:D:341:ARG:NH2[3_544]	2.15	0.05

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	252/709 (36%)	239 (95%)	10 (4%)	3 (1%)	10	20
1	B	388/709 (55%)	365 (94%)	21 (5%)	2 (0%)	24	43
1	C	246/709 (35%)	230 (94%)	16 (6%)	0	100	100
1	D	393/709 (55%)	366 (93%)	24 (6%)	3 (1%)	16	31
All	All	1279/2836 (45%)	1200 (94%)	71 (6%)	8 (1%)	21	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	SER
1	D	163	SER
1	A	15	ARG
1	A	59	ALA
1	B	153	GLY
1	D	164	ALA
1	B	154	ALA
1	A	191	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	196/556 (35%)	196 (100%)	0	100	100
1	B	306/556 (55%)	306 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	192/556 (34%)	190 (99%)	2 (1%)	68	86
1	D	306/556 (55%)	305 (100%)	1 (0%)	86	94
All	All	1000/2224 (45%)	997 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	198[A]	GLU
1	C	198[B]	GLU
1	D	63	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	B	42	GLN
1	B	64	ASN
1	B	342	HIS
1	C	12	ASN
1	C	92	HIS
1	C	104	ASN
1	D	26	ASN
1	D	94	GLN
1	D	260	HIS
1	D	317	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	144	B	502	-	1,7,7	0.38	0	3,9,9	2.86	2 (66%)
3	144	D	502	-	1,7,7	0.15	0	3,9,9	1.75	1 (33%)

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	144	B	502	-	-	0/0/9/9	-
3	144	D	502	-	-	0/0/9/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	144	C1-N-C2	-3.97	99.17	109.30
3	D	502	144	C1-N-C3	2.46	115.57	109.30
3	B	502	144	C1-N-C3	2.39	115.41	109.30

There are no chirality outliers.

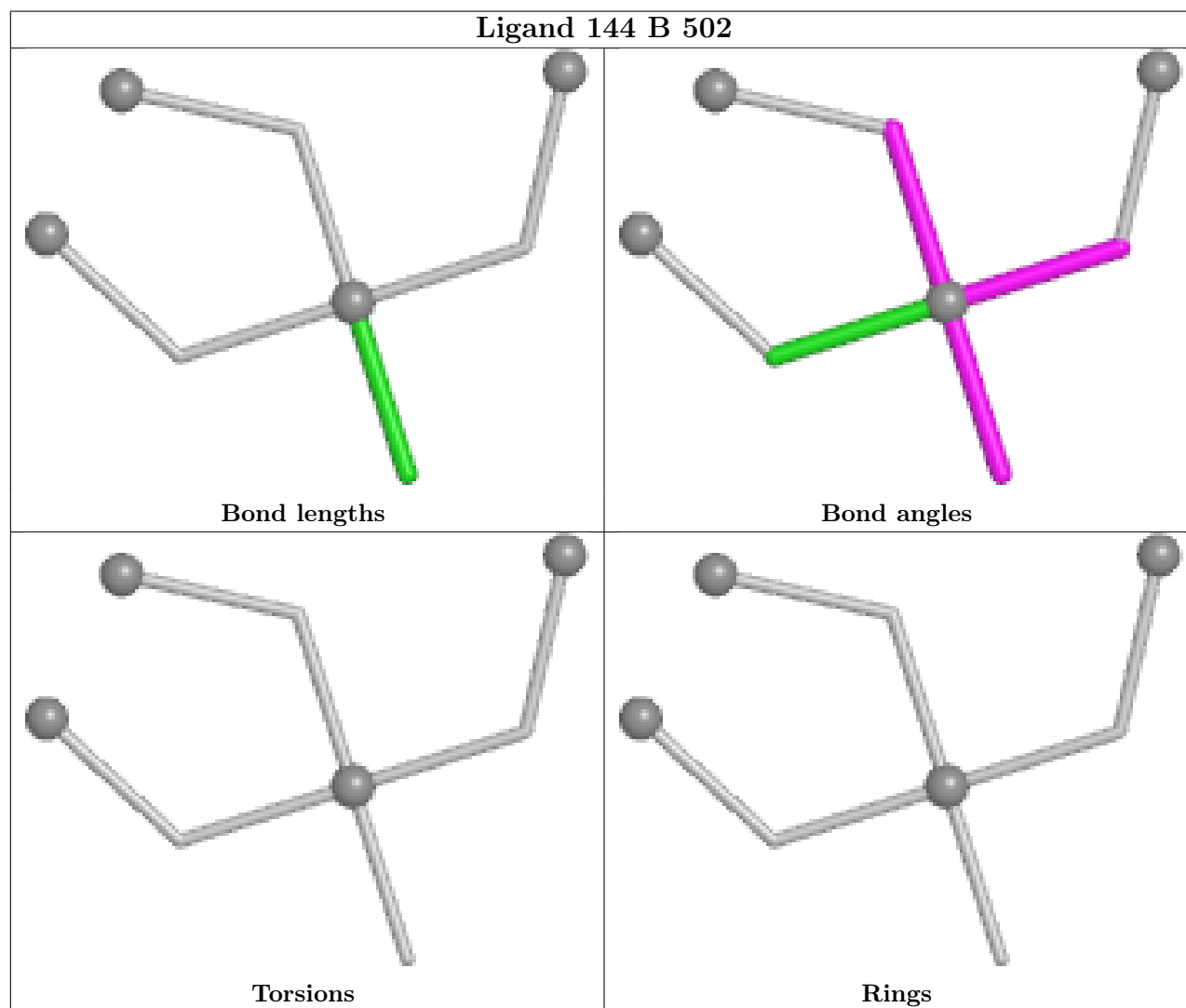
There are no torsion outliers.

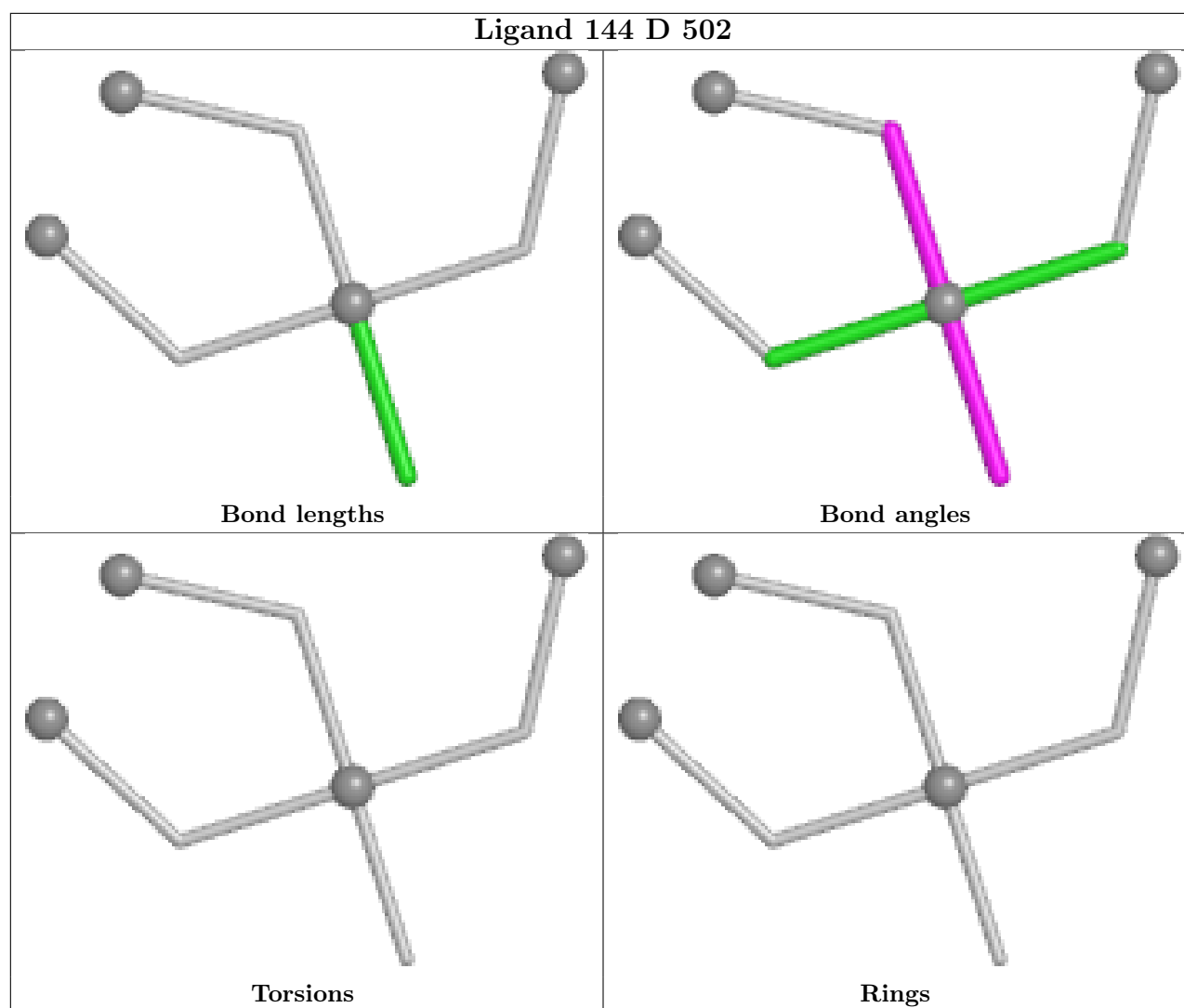
There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	144	14	0
3	D	502	144	10	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	256/709 (36%)	0.10	9 (3%)	47	42	44, 66, 91, 123	0
1	B	390/709 (55%)	0.04	5 (1%)	75	71	44, 59, 85, 109	0
1	C	249/709 (35%)	0.47	8 (3%)	50	46	41, 79, 98, 113	1 (0%)
1	D	394/709 (55%)	-0.05	7 (1%)	67	64	29, 59, 85, 105	1 (0%)
All	All	1289/2836 (45%)	0.11	29 (2%)	62	58	29, 64, 92, 123	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	ILE	5.4
1	A	268	ALA	4.7
1	C	198[A]	GLU	4.6
1	D	166	LEU	4.1
1	C	58	LEU	3.8
1	D	279	TYR	3.5
1	C	59	ALA	3.2
1	A	58	LEU	3.1
1	A	191	LEU	3.1
1	D	2	THR	2.9
1	D	164	ALA	2.8
1	A	190	ALA	2.8
1	A	1	MET	2.6
1	A	234	GLY	2.6
1	B	280	PHE	2.5
1	D	167	LYS	2.4
1	A	195	HIS	2.4
1	D	280	PHE	2.4
1	B	279	TYR	2.3
1	B	167	LYS	2.3
1	D	247	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.2
1	C	4	TYR	2.2
1	B	152	MET	2.1
1	C	60	ASP	2.1
1	A	193	LEU	2.1
1	B	153	GLY	2.1
1	C	216	SER	2.1
1	A	45	ALA	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

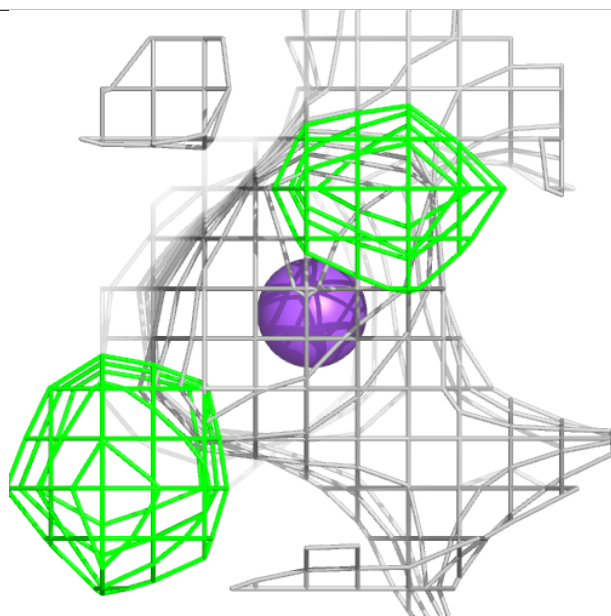
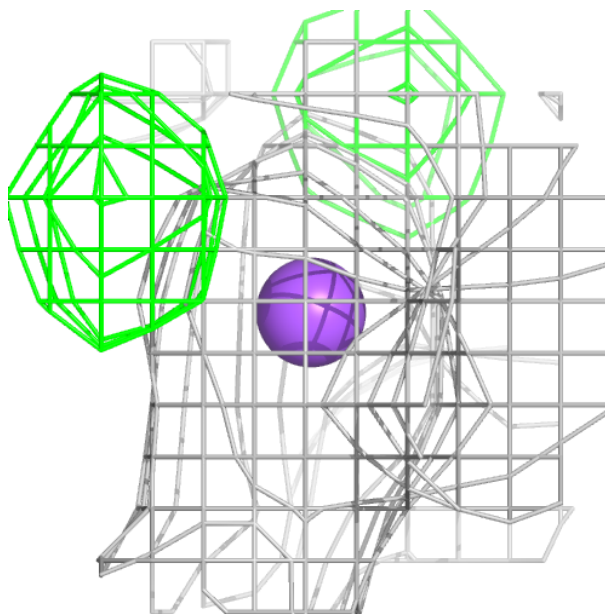
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	D	501	1/1	0.83	0.18	66,66,66,66	0
3	144	D	502	8/8	0.86	0.14	61,78,94,94	0
2	NA	B	501	1/1	0.87	0.18	65,65,65,65	0
3	144	B	502	8/8	0.89	0.12	57,62,67,67	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.

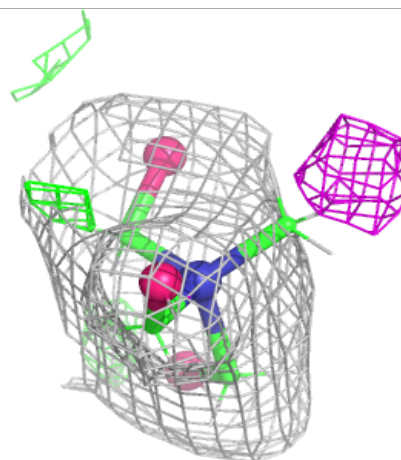
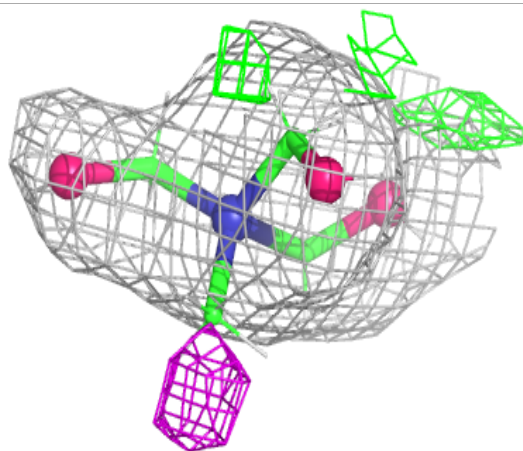
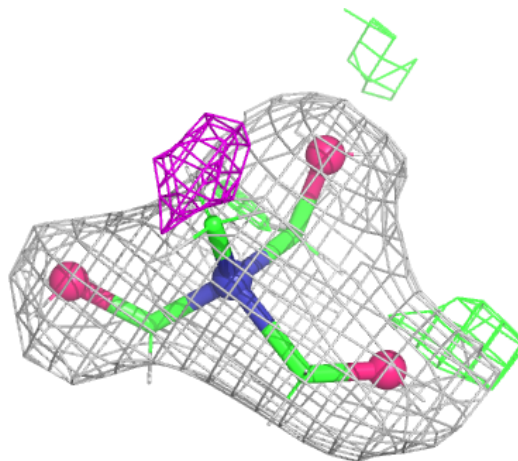
Electron density around NA D 501:

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



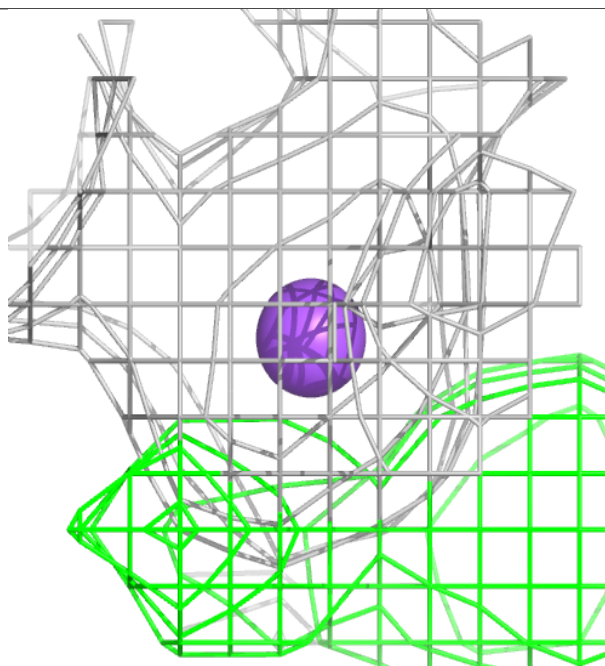
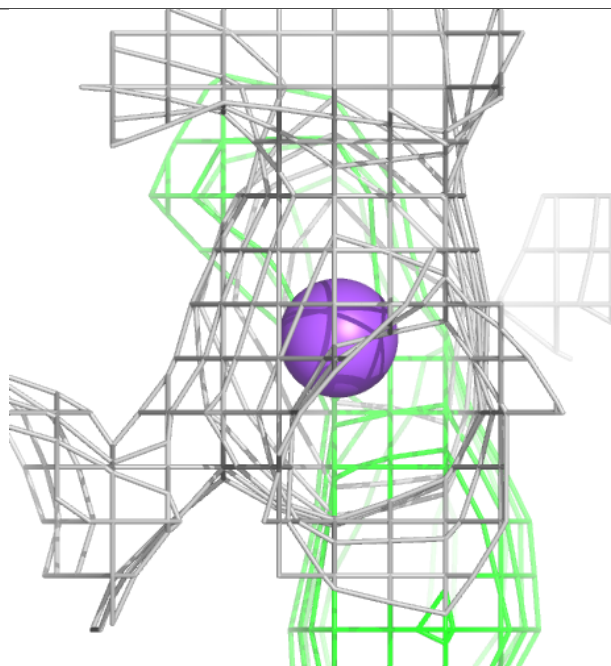
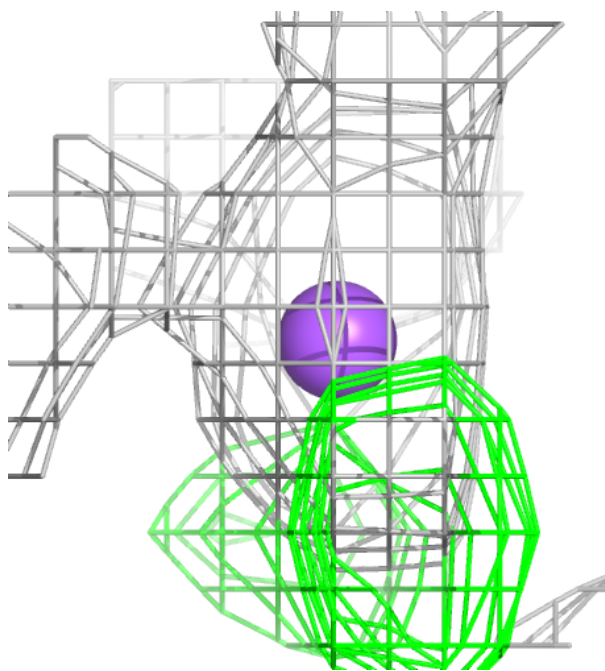
Electron density around 144 D 502:

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



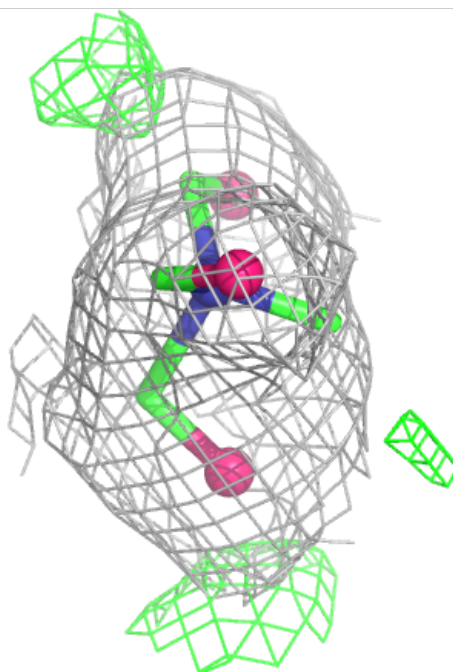
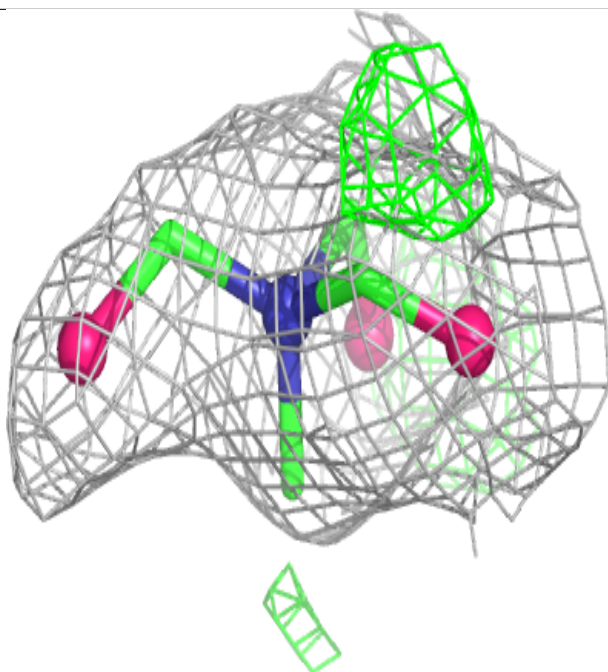
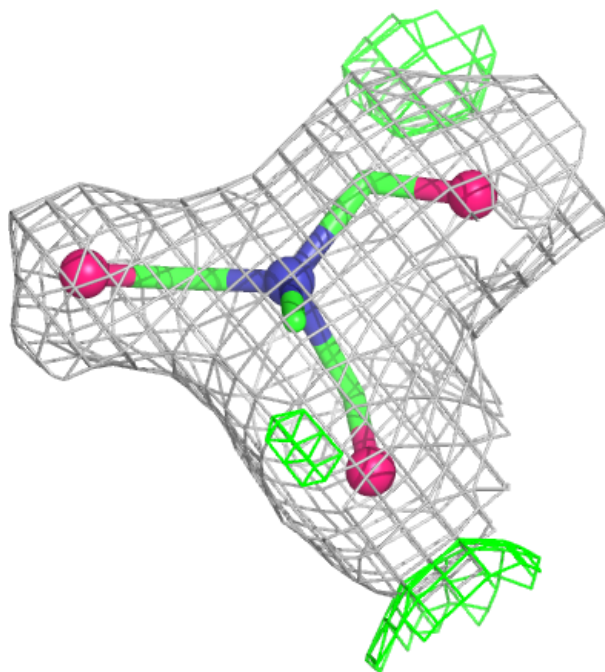
Electron density around NA B 501:

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



Electron density around 144 B 502:

$2mF_o-DF_c$ (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.