



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:29 AM UTC

PDB ID : 3MJS / pdb_00003mjs
Title : Structure of A-type Ketoreductases from Modular Polyketide Synthase
Authors : Zheng, J.; Taylor, C.A.; Piasecki, S.K.; Keatinge-Clay, A.T.
Deposited on : 2010-04-13
Resolution : 1.40 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

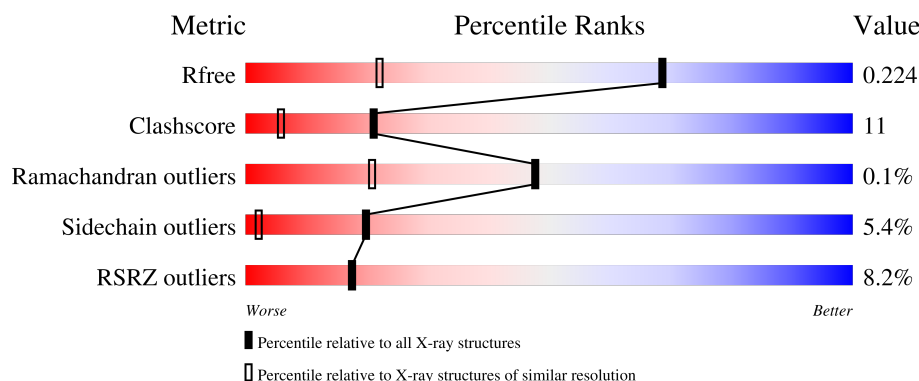
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	496	8% 73% 19% ...
1	B	496	8% 74% 17% ...

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	LMR	A	477	-	X	-	-
4	MLT	A	478	-	-	X	-
4	MLT	B	478	-	-	X	-
5	GOL	A	479	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7572 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 AmphB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3465	2163	635	658	9			
1	B	475	Total	C	N	O	S	0	0	0
			3459	2160	634	656	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q93NW7
A	-19	GLY	-	expression tag	UNP Q93NW7
A	-18	SER	-	expression tag	UNP Q93NW7
A	-17	SER	-	expression tag	UNP Q93NW7
A	-16	HIS	-	expression tag	UNP Q93NW7
A	-15	HIS	-	expression tag	UNP Q93NW7
A	-14	HIS	-	expression tag	UNP Q93NW7
A	-13	HIS	-	expression tag	UNP Q93NW7
A	-12	HIS	-	expression tag	UNP Q93NW7
A	-11	HIS	-	expression tag	UNP Q93NW7
A	-10	SER	-	expression tag	UNP Q93NW7
A	-9	SER	-	expression tag	UNP Q93NW7
A	-8	GLY	-	expression tag	UNP Q93NW7
A	-7	LEU	-	expression tag	UNP Q93NW7
A	-6	VAL	-	expression tag	UNP Q93NW7
A	-5	PRO	-	expression tag	UNP Q93NW7
A	-4	ARG	-	expression tag	UNP Q93NW7
A	-3	GLY	-	expression tag	UNP Q93NW7
A	-2	SER	-	expression tag	UNP Q93NW7
A	-1	HIS	-	expression tag	UNP Q93NW7
A	0	MET	-	expression tag	UNP Q93NW7
B	-20	MET	-	expression tag	UNP Q93NW7
B	-19	GLY	-	expression tag	UNP Q93NW7
B	-18	SER	-	expression tag	UNP Q93NW7
B	-17	SER	-	expression tag	UNP Q93NW7

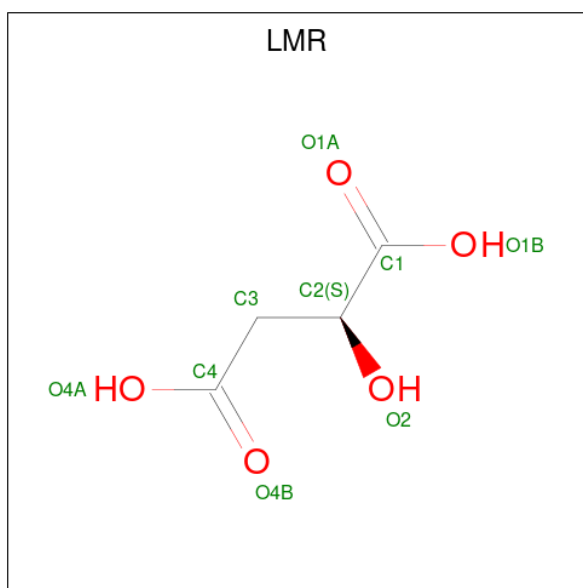
Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q93NW7
B	-15	HIS	-	expression tag	UNP Q93NW7
B	-14	HIS	-	expression tag	UNP Q93NW7
B	-13	HIS	-	expression tag	UNP Q93NW7
B	-12	HIS	-	expression tag	UNP Q93NW7
B	-11	HIS	-	expression tag	UNP Q93NW7
B	-10	SER	-	expression tag	UNP Q93NW7
B	-9	SER	-	expression tag	UNP Q93NW7
B	-8	GLY	-	expression tag	UNP Q93NW7
B	-7	LEU	-	expression tag	UNP Q93NW7
B	-6	VAL	-	expression tag	UNP Q93NW7
B	-5	PRO	-	expression tag	UNP Q93NW7
B	-4	ARG	-	expression tag	UNP Q93NW7
B	-3	GLY	-	expression tag	UNP Q93NW7
B	-2	SER	-	expression tag	UNP Q93NW7
B	-1	HIS	-	expression tag	UNP Q93NW7
B	0	MET	-	expression tag	UNP Q93NW7

-
- The chemical structure of NDP (Nucleoside Diphosphate) is shown, consisting of a sugar, a phosphate group, and a nucleobase. The sugar is a five-membered ring with an oxygen atom at the top. The phosphate group is attached to the sugar at the 5' position. The nucleobase is attached to the sugar at the 1' position. The structure is labeled with various atoms and groups, including NH₂, NH, N, C, O, P, and H. The sugar is a ribose derivative, and the phosphate group is a diphosphate. The nucleobase is a pyrimidine derivative.

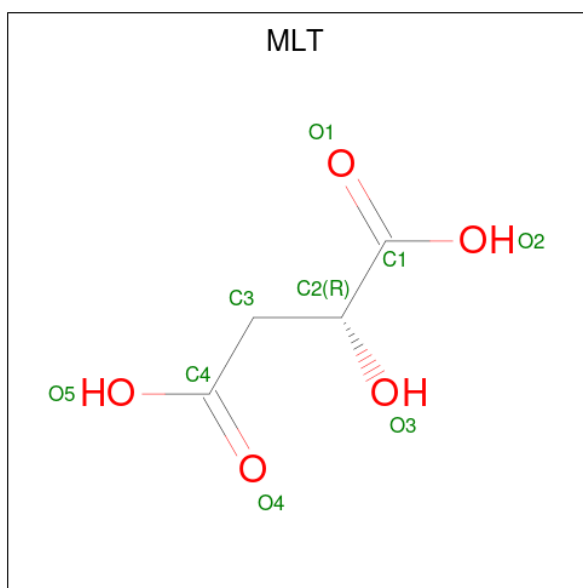
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		
4	B	1	Total	C	O	0	0
			9	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

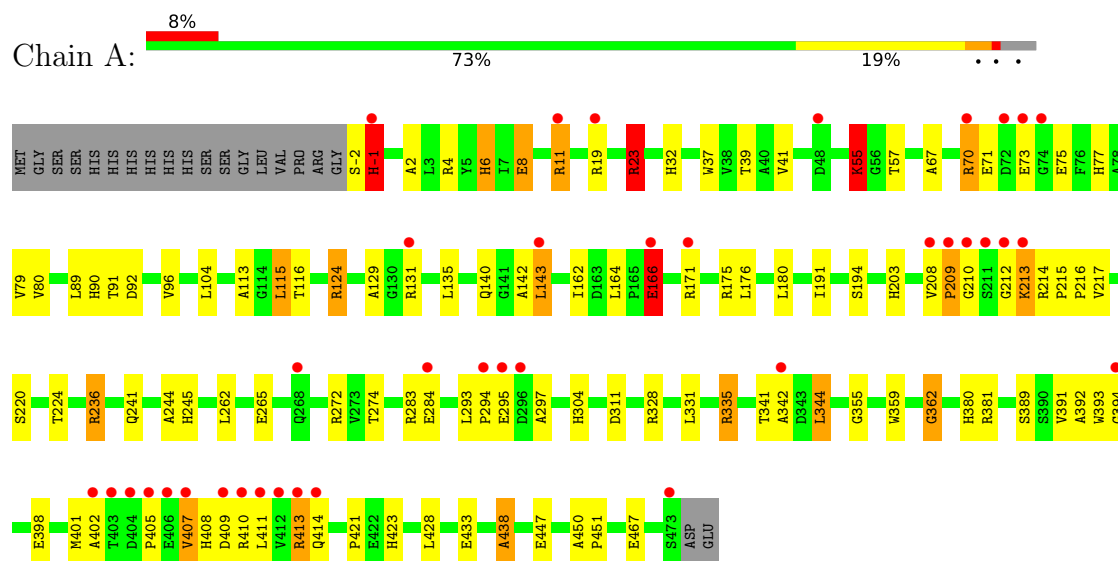
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	248	Total	O	0	0
			248	248		
6	B	256	Total	O	0	0
			256	256		

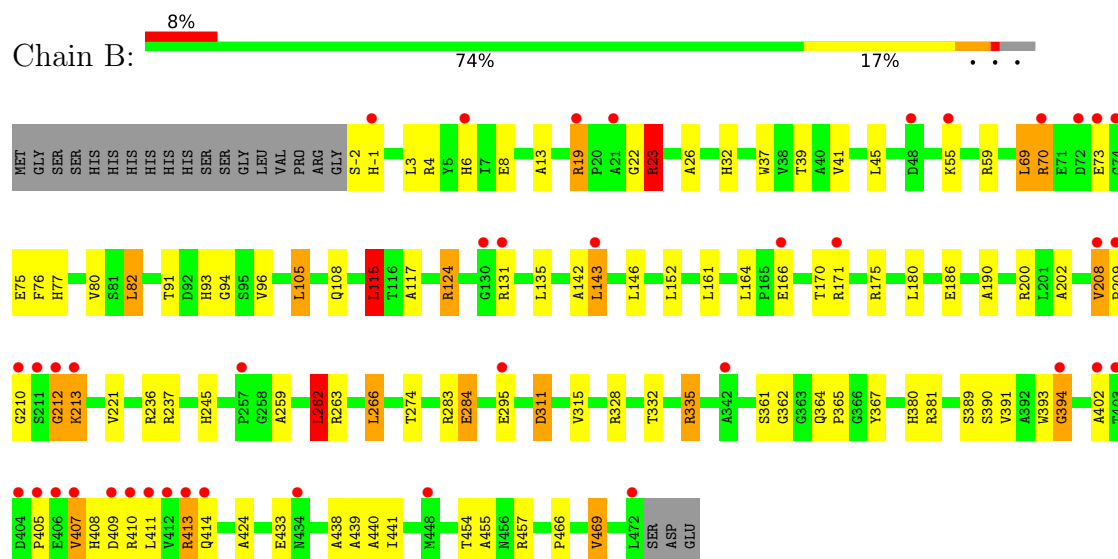
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: AmphB



• Molecule 1: AmphB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.44Å 63.71Å 71.82Å 72.77° 67.09° 89.79°	Depositor
Resolution (Å)	62.68 – 1.40 62.68 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (62.68-1.40) 94.7 (62.68-1.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.199 , 0.226 0.198 , 0.224	Depositor DCC
R_{free} test set	8865 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.083 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7572	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: LMR, NDP, GOL, MLT

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	1.84	47/3535 (1.3%)	1.54	31/4829 (0.6%)
1	B	1.86	49/3529 (1.4%)	1.59	38/4821 (0.8%)
All	All	1.85	96/7064 (1.4%)	1.56	69/9650 (0.7%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	LEU	C-N	16.93	1.57	1.33
1	B	94	GLY	C-N	9.99	1.47	1.33
1	A	208	VAL	C-O	9.63	1.35	1.24
1	B	143	LEU	N-CA	-9.55	1.34	1.46
1	B	166	GLU	C-O	9.51	1.36	1.24
1	B	70	ARG	C-N	9.43	1.46	1.33
1	A	71	GLU	C-N	-9.18	1.22	1.33
1	B	457	ARG	CB-CG	-8.58	1.26	1.52
1	A	166	GLU	CG-CD	-7.58	1.33	1.52
1	A	236	ARG	CB-CG	-7.53	1.29	1.52
1	A	389	SER	CB-OG	-7.50	1.27	1.42
1	A	394	GLY	C-O	7.32	1.33	1.23
1	A	32	HIS	CA-CB	7.21	1.58	1.53
1	A	362	GLY	CA-C	-7.20	1.45	1.52
1	A	115	LEU	C-N	-7.12	1.23	1.33
1	A	381	ARG	CA-C	-7.09	1.43	1.52
1	B	80	VAL	CA-CB	6.98	1.62	1.53
1	B	124	ARG	NE-CZ	6.95	1.40	1.33
1	A	162	ILE	N-CA	6.95	1.55	1.46
1	B	394	GLY	C-O	6.88	1.33	1.23
1	A	392	ALA	CA-CB	-6.79	1.44	1.53
1	A	209	PRO	CA-C	6.76	1.61	1.52
1	B	439	ALA	CA-C	-6.68	1.44	1.52
1	A	328	ARG	CD-NE	-6.64	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	ARG	CZ-NH2	-6.63	1.24	1.33
1	A	116	THR	C-N	-6.63	1.24	1.33
1	A	166	GLU	C-O	6.55	1.32	1.24
1	B	161	LEU	CA-C	-6.47	1.44	1.52
1	A	344	LEU	CG-CD1	-6.46	1.31	1.52
1	B	328	ARG	CD-NE	-6.45	1.37	1.46
1	B	26	ALA	C-O	6.42	1.31	1.23
1	B	262	LEU	CG-CD2	-6.41	1.31	1.52
1	A	297	ALA	CA-CB	-6.39	1.45	1.53
1	B	105	LEU	CG-CD1	-6.29	1.31	1.52
1	A	272	ARG	CZ-NH1	-6.28	1.24	1.32
1	B	457	ARG	N-CA	-6.12	1.36	1.46
1	A	6	HIS	CA-CB	-6.00	1.42	1.54
1	B	170	THR	CA-C	5.98	1.60	1.52
1	A	335	ARG	CZ-NH1	-5.89	1.24	1.32
1	A	129	ALA	C-O	-5.86	1.17	1.24
1	B	284	GLU	CB-CG	-5.84	1.34	1.52
1	A	96	VAL	CA-CB	-5.83	1.49	1.54
1	A	113	ALA	C-O	5.83	1.31	1.24
1	A	244	ALA	CA-CB	5.82	1.62	1.53
1	A	438	ALA	C-O	5.81	1.30	1.23
1	A	143	LEU	CG-CD2	-5.80	1.33	1.52
1	A	389	SER	CA-CB	-5.78	1.42	1.53
1	B	55	LYS	CB-CG	-5.78	1.35	1.52
1	A	294	PRO	CA-C	5.78	1.59	1.52
1	B	91	THR	CB-CG2	-5.74	1.33	1.52
1	B	166	GLU	CG-CD	-5.67	1.37	1.52
1	B	202	ALA	N-CA	5.66	1.53	1.45
1	A	208	VAL	CA-C	-5.61	1.48	1.53
1	A	450	ALA	N-CA	-5.59	1.41	1.46
1	B	213	LYS	N-CA	-5.58	1.39	1.46
1	B	76	PHE	CE1-CZ	-5.58	1.22	1.38
1	B	213	LYS	CA-C	-5.58	1.45	1.52
1	B	82	LEU	CG-CD1	-5.56	1.34	1.52
1	B	469	VAL	CB-CG2	-5.56	1.34	1.52
1	A	79	VAL	CA-CB	5.54	1.60	1.54
1	B	424	ALA	C-O	5.53	1.30	1.24
1	A	191	ILE	N-CA	5.52	1.52	1.46
1	A	104	LEU	N-CA	5.41	1.52	1.46
1	A	143	LEU	N-CA	-5.39	1.39	1.46
1	A	284	GLU	CB-CG	-5.37	1.36	1.52
1	A	80	VAL	CA-CB	5.36	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	VAL	CA-CB	-5.36	1.49	1.54
1	B	76	PHE	N-CA	5.36	1.52	1.45
1	B	4	ARG	N-CA	5.35	1.52	1.46
1	B	315	VAL	C-O	-5.33	1.17	1.24
1	A	142	ALA	CA-CB	5.32	1.62	1.53
1	B	441	ILE	CA-C	-5.31	1.45	1.52
1	B	389	SER	N-CA	5.30	1.52	1.46
1	B	186	GLU	N-CA	5.28	1.52	1.45
1	B	190	ALA	C-O	5.26	1.30	1.24
1	B	390	SER	CA-CB	-5.26	1.46	1.53
1	B	22	GLY	N-CA	5.21	1.51	1.45
1	B	146	LEU	C-O	5.18	1.30	1.24
1	B	209	PRO	C-O	5.17	1.29	1.23
1	A	23	ARG	CB-CG	-5.15	1.36	1.52
1	B	3	LEU	N-CA	5.11	1.52	1.46
1	B	455	ALA	CA-CB	-5.11	1.45	1.53
1	A	8	GLU	CD-OE1	-5.11	1.15	1.25
1	A	143	LEU	CG-CD1	-5.11	1.35	1.52
1	A	2	ALA	C-O	-5.09	1.17	1.24
1	A	39	THR	CA-CB	5.09	1.61	1.53
1	B	266	LEU	CG-CD1	-5.08	1.35	1.52
1	B	332	THR	C-O	5.08	1.30	1.24
1	B	381	ARG	CA-C	-5.08	1.46	1.52
1	A	342	ALA	C-O	5.07	1.29	1.24
1	B	440	ALA	CA-C	-5.06	1.46	1.52
1	B	221	VAL	N-CA	5.05	1.52	1.46
1	A	398	GLU	N-CA	5.05	1.52	1.46
1	B	335	ARG	CD-NE	-5.05	1.39	1.46
1	A	294	PRO	N-CA	5.04	1.52	1.47
1	B	93	HIS	C-O	5.01	1.29	1.23

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	VAL	CA-C-N	-12.24	107.52	119.76
1	B	208	VAL	C-N-CA	-12.24	107.52	119.76
1	B	212	GLY	CA-C-N	-10.29	105.85	123.25
1	B	212	GLY	C-N-CA	-10.29	105.85	123.25
1	B	210	GLY	N-CA-C	9.95	128.14	115.21
1	B	335	ARG	NE-CZ-NH2	9.42	127.68	119.20
1	A	19	ARG	NE-CZ-NH2	9.39	127.65	119.20
1	A	241	GLN	N-CA-C	9.02	124.09	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH1	-8.97	112.53	121.50
1	A	335	ARG	NE-CZ-NH2	8.89	127.20	119.20
1	A	293	LEU	N-CA-C	8.72	119.63	109.60
1	A	55	LYS	CD-CE-NZ	-8.40	85.01	111.90
1	A	284	GLU	CB-CG-CD	-8.19	98.68	112.60
1	A	208	VAL	O-C-N	7.89	128.18	120.92
1	A	328	ARG	CG-CD-NE	-7.70	95.05	112.00
1	B	94	GLY	O-C-N	7.69	131.37	122.68
1	A	328	ARG	NE-CZ-NH2	7.68	126.11	119.20
1	A	166	GLU	CB-CG-CD	-7.62	99.65	112.60
1	B	55	LYS	CD-CE-NZ	-7.55	87.73	111.90
1	B	414	GLN	N-CA-CB	-7.49	98.99	110.44
1	A	335	ARG	NE-CZ-NH1	-7.29	114.21	121.50
1	B	335	ARG	NE-CZ-NH1	-7.28	114.22	121.50
1	B	19	ARG	NE-CZ-NH2	7.14	125.63	119.20
1	B	82	LEU	CB-CG-CD1	7.12	132.07	110.70
1	B	124	ARG	NE-CZ-NH2	7.04	125.53	119.20
1	B	213	LYS	N-CA-C	-7.04	101.24	111.30
1	A	166	GLU	N-CA-CB	6.87	120.88	110.30
1	B	259	ALA	N-CA-C	6.67	118.56	111.28
1	B	19	ARG	CA-C-N	-6.67	112.89	119.76
1	B	19	ARG	C-N-CA	-6.67	112.89	119.76
1	A	176	LEU	CB-CG-CD1	6.63	130.58	110.70
1	A	344	LEU	CD1-CG-CD2	-6.27	97.00	110.80
1	B	200	ARG	NE-CZ-NH1	6.01	127.52	121.50
1	B	284	GLU	CB-CG-CD	-6.01	102.38	112.60
1	B	263	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	A	115	LEU	CD1-CG-CD2	-5.85	97.93	110.80
1	A	210	GLY	N-CA-C	5.79	123.32	115.32
1	B	94	GLY	CA-C-N	-5.74	113.47	122.65
1	B	94	GLY	C-N-CA	-5.74	113.47	122.65
1	A	272	ARG	NE-CZ-NH2	5.71	124.33	119.20
1	B	367	TYR	N-CA-CB	-5.65	101.53	110.28
1	A	19	ARG	CG-CD-NE	-5.64	99.58	112.00
1	A	70	ARG	O-C-N	5.64	129.99	122.43
1	A	214	ARG	NE-CZ-NH2	-5.63	114.14	119.20
1	A	115	LEU	CB-CG-CD1	-5.62	93.83	110.70
1	B	236	ARG	CB-CG-CD	-5.58	98.47	111.30
1	A	71	GLU	CA-C-N	5.56	127.73	120.28
1	A	71	GLU	C-N-CA	5.56	127.73	120.28
1	B	328	ARG	CB-CG-CD	-5.56	98.51	111.30
1	A	176	LEU	N-CA-C	5.52	116.99	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LEU	CD1-CG-CD2	-5.50	98.70	110.80
1	A	4	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	A	143	LEU	O-C-N	-5.39	115.64	122.27
1	B	209	PRO	CA-C-O	-5.34	114.91	121.31
1	A	19	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	B	23	ARG	CA-CB-CG	-5.21	103.67	114.10
1	B	166	GLU	CB-CG-CD	-5.19	103.78	112.60
1	B	469	VAL	CG1-CB-CG2	-5.13	99.51	110.80
1	B	142	ALA	O-C-N	-5.12	116.23	122.22
1	B	115	LEU	CB-CG-CD1	-5.11	95.37	110.70
1	B	55	LYS	CB-CA-C	-5.10	101.33	109.75
1	B	414	GLN	CA-CB-CG	5.10	124.30	114.10
1	B	117	ALA	N-CA-C	-5.10	103.36	109.83
1	A	209	PRO	CB-CA-C	5.08	119.94	111.56
1	B	39	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	71	GLU	N-CA-C	-5.04	104.73	111.24
1	A	-1	HIS	CB-CA-C	5.04	119.16	110.79
1	B	454	THR	O-C-N	5.03	128.44	122.26
1	A	166	GLU	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

There are no planarity outliers.

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	3465	0	3426	83	1
1	B	3459	0	3421	80	1
2	A	48	0	26	1	0
2	B	48	0	26	1	0
3	A	9	0	4	0	0
4	A	9	0	4	4	0
4	B	18	0	8	5	0
5	A	6	0	8	6	0
5	B	6	0	8	2	0
6	A	248	0	0	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	256	0	0	9	0
All	All	7572	0	6931	154	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (154) 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:212:GLY:CA	1:B:433:GLU:O	1.92	1.18
1:A:11:ARG:HH21	1:A:11:ARG:HG3	1.14	1.12
1:A:11:ARG:NH1	1:A:194:SER:O	1.86	1.07
1:B:212:GLY:HA3	1:B:433:GLU:O	1.50	1.07
1:A:217:VAL:H	5:A:479:GOL:H11	1.21	1.00
1:A:341:THR:HA	1:A:344:LEU:HD13	1.42	1.00
1:B:469:VAL:HB	6:B:654:HOH:O	0.82	0.99
1:B:212:GLY:HA2	1:B:433:GLU:O	1.62	0.99
1:A:209:PRO:O	6:A:708:HOH:O	1.81	0.99
1:B:237:ARG:HG2	5:B:479:GOL:O2	1.65	0.95
1:A:212:GLY:HA3	1:A:433:GLU:O	1.64	0.94
1:A:11:ARG:HH21	1:A:11:ARG:CG	1.82	0.93
1:B:262:LEU:O	1:B:266:LEU:HD13	1.69	0.93
1:A:90:HIS:HD2	1:A:92:ASP:H	1.14	0.91
1:A:-1:HIS:NE2	1:A:423:HIS:CD2	2.41	0.89
1:A:-1:HIS:NE2	1:A:423:HIS:CG	2.44	0.85
1:A:217:VAL:H	5:A:479:GOL:C1	1.89	0.84
1:A:362:GLY:H	4:A:478:MLT:H32	1.43	0.83
1:A:11:ARG:HG3	1:A:11:ARG:NH2	1.81	0.81
1:A:402:ALA:HA	1:A:407:VAL:CG1	2.11	0.81
1:B:23:ARG:NH1	1:B:73:GLU:OE1	2.13	0.81
1:B:402:ALA:HA	1:B:407:VAL:CG1	2.10	0.81
1:A:217:VAL:N	5:A:479:GOL:H11	1.96	0.79
1:B:262:LEU:HD23	1:B:266:LEU:HD13	1.65	0.79
1:A:209:PRO:CD	1:B:13:ALA:HB2	2.13	0.78
1:A:209:PRO:HD2	1:B:13:ALA:CB	2.15	0.77
1:A:236:ARG:HG2	1:A:265:GLU:OE2	1.84	0.77
1:A:212:GLY:CA	1:A:433:GLU:O	2.33	0.75
1:A:209:PRO:HG2	1:B:13:ALA:HB2	1.69	0.75
1:A:362:GLY:H	4:A:478:MLT:C3	2.00	0.74
1:B:59:ARG:HB2	1:B:105:LEU:HD12	1.69	0.73
1:A:209:PRO:HD2	1:B:13:ALA:HB2	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD23	1:B:266:LEU:CD1	2.18	0.73
1:B:73:GLU:HG2	6:B:708:HOH:O	1.86	0.72
1:A:-1:HIS:CE1	1:A:423:HIS:CE1	2.78	0.72
1:A:245:HIS:HE1	1:A:274:THR:OG1	1.73	0.72
1:A:203:HIS:HE1	1:A:467:GLU:OE2	1.71	0.71
1:A:6:HIS:NE2	1:A:8:GLU:OE2	2.25	0.69
1:A:209:PRO:CG	1:B:13:ALA:HB2	2.22	0.69
1:A:90:HIS:CD2	1:A:92:ASP:H	2.05	0.69
1:B:73:GLU:OE1	6:B:708:HOH:O	2.09	0.68
1:B:466:PRO:O	1:B:469:VAL:HG23	1.93	0.67
1:B:413:ARG:HH11	1:B:413:ARG:HG3	1.59	0.67
1:B:19:ARG:HH11	1:B:19:ARG:CB	2.08	0.67
1:A:203:HIS:HD2	6:A:549:HOH:O	1.78	0.67
1:A:236:ARG:NE	1:A:265:GLU:OE2	2.28	0.67
1:B:466:PRO:HA	1:B:469:VAL:CG2	2.27	0.65
1:A:391:VAL:HG21	1:A:428:LEU:HD13	1.80	0.64
1:A:209:PRO:HD2	1:B:13:ALA:CA	2.29	0.63
1:B:41:VAL:CG2	1:B:164:LEU:HD11	2.29	0.63
1:B:19:ARG:HH11	1:B:19:ARG:HB2	1.63	0.62
1:B:32:HIS:HE1	6:B:699:HOH:O	1.82	0.62
1:B:41:VAL:HG21	1:B:164:LEU:HD11	1.80	0.62
1:B:237:ARG:HG2	5:B:479:GOL:C2	2.30	0.62
1:B:19:ARG:CB	1:B:19:ARG:NH1	2.63	0.62
1:B:245:HIS:HE1	1:B:274:THR:OG1	1.81	0.61
1:B:19:ARG:NH1	1:B:19:ARG:HB3	2.15	0.61
1:A:209:PRO:HD2	1:B:13:ALA:HA	1.81	0.61
1:A:55:LYS:HD3	6:A:512:HOH:O	2.00	0.61
1:B:19:ARG:NH2	1:B:45:LEU:O	2.32	0.61
1:A:216:PRO:HA	5:A:479:GOL:H11	1.82	0.61
1:B:262:LEU:HD23	1:B:262:LEU:C	2.26	0.61
1:A:236:ARG:CG	1:A:265:GLU:OE2	2.49	0.60
1:B:402:ALA:HA	1:B:407:VAL:HG11	1.82	0.60
1:A:166:GLU:OE2	1:A:166:GLU:CA	2.48	0.60
1:A:77:HIS:HE1	1:A:180:LEU:O	1.84	0.60
1:A:124:ARG:HD2	1:A:166:GLU:HA	1.84	0.59
1:A:212:GLY:N	1:A:433:GLU:O	2.36	0.58
1:A:402:ALA:HA	1:A:407:VAL:HG11	1.83	0.58
1:A:405:PRO:O	1:A:409:ASP:OD2	2.20	0.58
1:B:361:SER:HA	4:B:478:MLT:H2	1.85	0.58
1:A:-1:HIS:NE2	1:A:423:HIS:CE1	2.71	0.58
1:A:-1:HIS:CE1	1:A:423:HIS:ND1	2.73	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ARG:NH2	6:B:553:HOH:O	1.98	0.57
1:A:209:PRO:HG2	1:B:13:ALA:CB	2.34	0.56
1:A:124:ARG:H	1:A:140:GLN:NE2	2.03	0.56
1:B:73:GLU:CG	6:B:708:HOH:O	2.49	0.56
1:B:23:ARG:HH11	1:B:73:GLU:CD	2.14	0.55
1:B:212:GLY:HA3	1:B:433:GLU:C	2.30	0.55
1:A:-1:HIS:NE2	1:A:423:HIS:NE2	2.54	0.55
1:B:37:TRP:CD1	1:B:124:ARG:HG2	2.41	0.54
1:B:59:ARG:HB2	1:B:105:LEU:CD1	2.38	0.54
1:B:77:HIS:HE1	1:B:180:LEU:O	1.90	0.53
1:B:135:LEU:O	1:B:380:HIS:HD2	1.91	0.53
1:A:220:SER:OG	1:A:245:HIS:HD2	1.91	0.53
1:A:67:ALA:O	1:A:70:ARG:HG3	2.08	0.53
1:B:262:LEU:CD2	1:B:266:LEU:CD1	2.87	0.53
1:A:410:ARG:HG3	1:A:411:LEU:HD23	1.92	0.52
1:A:401:MET:O	1:A:407:VAL:HG11	2.09	0.52
1:A:341:THR:HA	1:A:344:LEU:CD1	2.29	0.52
1:B:438:ALA:HB2	6:B:525:HOH:O	2.09	0.51
1:B:262:LEU:C	1:B:262:LEU:CD2	2.83	0.51
1:B:171:ARG:HG2	1:B:175:ARG:NH1	2.26	0.51
1:B:407:VAL:O	1:B:411:LEU:HG	2.10	0.51
1:B:466:PRO:O	1:B:469:VAL:CG2	2.59	0.51
1:A:402:ALA:O	1:A:408:HIS:HB2	2.10	0.51
1:B:41:VAL:CG2	1:B:164:LEU:CD1	2.89	0.51
1:A:224:THR:OG1	1:A:304:HIS:HD2	1.94	0.50
1:B:402:ALA:HA	1:B:407:VAL:HG12	1.91	0.50
1:B:152:LEU:HD13	4:B:478:MLT:H31	1.94	0.50
1:A:-2:SER:N	6:A:692:HOH:O	2.27	0.50
1:B:105:LEU:HD13	1:B:108:GLN:OE1	2.12	0.50
1:B:262:LEU:O	1:B:262:LEU:HD23	2.11	0.50
1:B:41:VAL:HG21	1:B:164:LEU:CD1	2.42	0.49
1:B:413:ARG:HH11	1:B:413:ARG:CG	2.23	0.49
1:A:341:THR:CA	1:A:344:LEU:HD13	2.30	0.49
1:A:23:ARG:HH11	1:A:73:GLU:CD	2.20	0.49
1:A:393:TRP:HB2	2:A:476:NDP:C5N	2.43	0.49
1:B:469:VAL:CB	6:B:654:HOH:O	1.72	0.49
1:A:124:ARG:H	1:A:140:GLN:HE22	1.60	0.48
1:B:409:ASP:O	1:B:413:ARG:HB2	2.12	0.48
1:B:73:GLU:CD	6:B:708:HOH:O	2.56	0.48
1:B:393:TRP:HB2	2:B:476:NDP:C5N	2.44	0.48
1:A:283:ARG:NH1	6:A:679:HOH:O	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:THR:OG1	1:A:304:HIS:CD2	2.67	0.47
1:A:57:THR:OG1	1:A:90:HIS:HE1	1.97	0.47
1:B:362:GLY:H	4:B:478:MLT:C3	2.28	0.47
1:B:410:ARG:HG3	1:B:411:LEU:HD23	1.98	0.46
1:B:6:HIS:CD2	1:B:8:GLU:HG3	2.50	0.46
1:A:91:THR:HG22	6:A:527:HOH:O	2.15	0.46
1:B:262:LEU:CD2	1:B:266:LEU:HD11	2.46	0.46
1:B:70:ARG:HB2	1:B:115:LEU:HD11	1.98	0.46
1:A:37:TRP:CE2	1:A:124:ARG:HB2	2.51	0.45
1:A:362:GLY:N	4:A:478:MLT:H32	2.23	0.45
1:A:41:VAL:HG21	1:A:164:LEU:HD11	1.99	0.45
1:B:466:PRO:HA	1:B:469:VAL:HG22	1.97	0.45
1:A:355:GLY:HA3	1:A:359:TRP:CZ2	2.52	0.44
1:B:402:ALA:O	1:B:408:HIS:HB2	2.17	0.44
1:B:69:LEU:O	1:B:73:GLU:HB2	2.16	0.44
1:B:266:LEU:HD12	1:B:266:LEU:N	2.32	0.44
1:A:135:LEU:O	1:A:380:HIS:HD2	2.00	0.44
1:A:438:ALA:HB2	6:A:674:HOH:O	2.17	0.44
1:A:37:TRP:CG	1:A:124:ARG:HG3	2.52	0.44
1:A:89:LEU:HD11	1:A:335:ARG:HH22	1.81	0.43
1:A:391:VAL:HG21	1:A:428:LEU:CD1	2.46	0.43
1:A:209:PRO:CG	1:B:13:ALA:CB	2.94	0.43
1:A:283:ARG:NE	6:A:679:HOH:O	2.13	0.43
1:A:409:ASP:O	1:A:413:ARG:HB2	2.18	0.43
1:A:171:ARG:HG2	1:A:175:ARG:NH1	2.34	0.43
1:A:212:GLY:C	1:A:213:LYS:HG3	2.44	0.42
1:B:405:PRO:O	1:B:409:ASP:OD2	2.36	0.42
1:B:362:GLY:H	4:B:478:MLT:H2	1.84	0.42
1:A:236:ARG:CD	1:A:265:GLU:OE2	2.67	0.42
1:A:215:PRO:O	5:A:479:GOL:H31	2.20	0.42
1:B:6:HIS:CD2	1:B:6:HIS:C	2.97	0.42
1:B:413:ARG:HG3	1:B:413:ARG:NH1	2.28	0.42
1:A:331:LEU:C	1:A:331:LEU:HD23	2.45	0.42
1:A:-1:HIS:NE2	1:A:423:HIS:ND1	2.65	0.42
1:A:414:GLN:CD	4:A:478:MLT:O3	2.64	0.41
1:B:6:HIS:HD2	1:B:8:GLU:HG3	1.86	0.41
1:B:362:GLY:H	4:B:478:MLT:C2	2.34	0.41
1:B:262:LEU:CD2	1:B:266:LEU:HD13	2.44	0.40
1:A:216:PRO:CA	5:A:479:GOL:H11	2.50	0.40
1:B:364:GLN:N	1:B:365:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:NH1	1:B:311:ASP:OD1[1_664]	1.92	0.28

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	474/496 (96%)	465 (98%)	9 (2%)	0	100	100
1	B	473/496 (95%)	464 (98%)	8 (2%)	1 (0%)	43	19
All	All	947/992 (96%)	929 (98%)	17 (2%)	1 (0%)	48	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	394	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/351 (95%)	315 (94%)	19 (6%)	18	2
1	B	333/351 (95%)	316 (95%)	17 (5%)	21	3
All	All	667/702 (95%)	631 (95%)	36 (5%)	20	2

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	11	ARG
1	A	23	ARG
1	A	55	LYS
1	A	75	GLU
1	A	115	LEU
1	A	124	ARG
1	A	131	ARG
1	A	143	LEU
1	A	166	GLU
1	A	213	LYS
1	A	262	LEU
1	A	295	GLU
1	A	311	ASP
1	A	407	VAL
1	A	413	ARG
1	A	421	PRO
1	A	447	GLU
1	A	451	PRO
1	B	-2	SER
1	B	-1	HIS
1	B	23	ARG
1	B	75	GLU
1	B	82	LEU
1	B	115	LEU
1	B	131	ARG
1	B	143	LEU
1	B	208	VAL
1	B	213	LYS
1	B	262	LEU
1	B	284	GLU
1	B	295	GLU
1	B	311	ASP
1	B	391	VAL
1	B	407	VAL
1	B	413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	68	GLN
1	A	77	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	90	HIS
1	A	140	GLN
1	A	203	HIS
1	A	241	GLN
1	A	245	HIS
1	A	304	HIS
1	A	336	HIS
1	A	380	HIS
1	A	414	GLN
1	B	32	HIS
1	B	68	GLN
1	B	77	HIS
1	B	241	GLN
1	B	245	HIS
1	B	380	HIS
1	B	434	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	LMR	A	477	-	8,8,8	2.37	4 (50%)	10,10,10	3.01	5 (50%)
5	GOL	A	479	-	5,5,5	1.31	1 (20%)	5,5,5	1.40	2 (40%)
2	NDP	A	476	-	51,52,52	1.89	14 (27%)	71,80,80	1.70	14 (19%)
4	MLT	B	478	-	8,8,8	1.76	3 (37%)	10,10,10	2.51	4 (40%)
2	NDP	B	476	-	51,52,52	1.56	11 (21%)	71,80,80	1.68	15 (21%)
4	MLT	B	477	-	8,8,8	1.25	1 (12%)	10,10,10	2.42	4 (40%)
5	GOL	B	479	-	5,5,5	0.54	0	5,5,5	0.90	0
4	MLT	A	478	-	8,8,8	1.20	1 (12%)	10,10,10	2.72	6 (60%)

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	LMR	A	477	-	-	4/8/8/8	-
5	GOL	A	479	-	-	4/4/4/4	-
2	NDP	A	476	-	-	5/34/77/77	0/5/5/5
4	MLT	B	478	-	-	2/8/8/8	-
2	NDP	B	476	-	-	7/34/77/77	0/5/5/5
4	MLT	B	477	-	-	3/8/8/8	-
5	GOL	B	479	-	-	0/4/4/4	-
4	MLT	A	478	-	-	3/8/8/8	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	476	NDP	PA-O3	5.05	1.64	1.59
2	A	476	NDP	PN-O3	-4.86	1.54	1.59
3	A	477	LMR	C2-C1	-4.56	1.45	1.52
2	B	476	NDP	C4N-C5N	-4.26	1.38	1.49
2	A	476	NDP	C4N-C5N	-4.10	1.38	1.49
2	A	476	NDP	C3B-C4B	-3.80	1.43	1.53
2	A	476	NDP	C8A-N7A	3.68	1.38	1.31
2	B	476	NDP	C4N-C3N	-3.64	1.43	1.50
2	A	476	NDP	C6N-C5N	3.44	1.43	1.33
3	A	477	LMR	O1B-C1	-3.08	1.20	1.30
2	A	476	NDP	P2B-O2B	3.02	1.64	1.59
2	A	476	NDP	C2D-C3D	-2.97	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	476	NDP	C4N-C3N	-2.93	1.44	1.50
4	B	478	MLT	C2-C1	2.87	1.56	1.52
2	B	476	NDP	O4D-C1D	2.82	1.48	1.42
2	B	476	NDP	PN-O3	-2.77	1.56	1.59
2	B	476	NDP	C8A-N7A	2.76	1.37	1.31
2	A	476	NDP	P2B-O2X	-2.70	1.44	1.54
2	A	476	NDP	C8A-N9A	-2.68	1.33	1.37
2	B	476	NDP	PA-O3	2.66	1.62	1.59
4	B	478	MLT	O1-C1	2.58	1.29	1.22
3	A	477	LMR	O2-C2	-2.53	1.37	1.42
2	B	476	NDP	C3B-C4B	-2.42	1.46	1.53
3	A	477	LMR	O4A-C4	-2.39	1.22	1.30
2	B	476	NDP	O4B-C4B	-2.34	1.39	1.45
4	B	478	MLT	C3-C2	2.28	1.57	1.52
4	A	478	MLT	C3-C4	2.28	1.57	1.51
4	B	477	MLT	O5-C4	-2.24	1.23	1.30
2	B	476	NDP	C3D-C4D	2.24	1.58	1.53
2	B	476	NDP	P2B-O2X	-2.15	1.46	1.54
2	A	476	NDP	C2N-C3N	2.14	1.41	1.35
2	A	476	NDP	O4D-C1D	2.13	1.46	1.42
2	A	476	NDP	O3B-C3B	2.11	1.48	1.43
5	A	479	GOL	C3-C2	2.10	1.59	1.51
2	B	476	NDP	PN-O2N	-2.07	1.45	1.55

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	476	NDP	N3A-C2A-N1A	-5.61	120.10	128.58
3	A	477	LMR	O1A-C1-C2	-5.18	112.26	122.60
3	A	477	LMR	O2-C2-C1	-5.14	97.30	110.36
3	A	477	LMR	O1B-C1-C2	4.87	123.04	112.74
4	B	478	MLT	C2-C3-C4	4.84	124.72	112.08
2	A	476	NDP	N9A-C8A-N7A	-4.79	107.14	113.94
4	A	478	MLT	O1-C1-C2	-4.78	113.06	122.60
2	A	476	NDP	C4A-C5A-N7A	-4.64	105.28	110.58
4	B	478	MLT	C3-C2-C1	4.35	121.20	110.53
4	A	478	MLT	O2-C1-C2	4.24	121.70	112.74
2	A	476	NDP	C5A-N7A-C8A	4.04	109.80	103.45
4	B	477	MLT	C2-C3-C4	4.01	122.57	112.08
2	B	476	NDP	C2A-N1A-C6A	3.92	125.17	118.73
4	B	477	MLT	O2-C1-C2	3.84	120.86	112.74
2	B	476	NDP	O2B-P2B-O1X	-3.40	97.20	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	O2B-P2B-O1X	-3.35	97.38	109.33
2	A	476	NDP	C2B-C1B-N9A	3.33	119.23	113.75
2	B	476	NDP	C3N-C2N-N1N	-3.14	118.60	123.20
4	A	478	MLT	C2-C3-C4	3.06	120.08	112.08
2	A	476	NDP	N3A-C2A-N1A	-3.05	123.97	128.58
4	B	477	MLT	O1-C1-C2	-3.01	116.58	122.60
2	B	476	NDP	O4B-C4B-C3B	3.00	111.12	105.15
2	B	476	NDP	N9A-C8A-N7A	-2.93	109.78	113.94
2	B	476	NDP	N6A-C6A-N1A	2.89	124.82	118.38
4	A	478	MLT	O3-C2-C1	-2.89	103.02	110.36
2	A	476	NDP	C5A-C4A-N9A	2.88	108.95	105.81
3	A	477	LMR	C3-C2-C1	2.86	117.55	110.53
2	A	476	NDP	C4A-N9A-C8A	2.86	108.74	105.74
2	A	476	NDP	O4B-C4B-C3B	2.85	110.81	105.15
2	B	476	NDP	C6N-N1N-C2N	2.78	122.29	119.32
4	B	477	MLT	O3-C2-C1	-2.72	103.46	110.36
4	A	478	MLT	O5-C4-C3	2.70	122.38	114.00
2	A	476	NDP	O4D-C1D-C2D	-2.60	101.05	106.62
2	A	476	NDP	C6A-C5A-N7A	2.51	136.93	132.09
4	B	478	MLT	O2-C1-O1	-2.47	118.47	124.08
4	A	478	MLT	O5-C4-O4	-2.43	117.09	123.33
4	B	478	MLT	O5-C4-C3	2.38	121.39	114.00
2	B	476	NDP	O3-PN-O1N	-2.36	103.62	110.70
2	B	476	NDP	O3B-C3B-C4B	-2.29	104.50	111.08
5	A	479	GOL	C3-C2-C1	2.28	120.14	111.80
2	B	476	NDP	C4A-C5A-N7A	-2.24	108.02	110.58
2	A	476	NDP	C3N-C2N-N1N	-2.19	119.98	123.20
2	B	476	NDP	C5A-N7A-C8A	2.16	106.85	103.45
2	A	476	NDP	C4B-O4B-C1B	-2.14	104.73	109.47
2	B	476	NDP	C5A-C4A-N9A	2.12	108.12	105.81
2	A	476	NDP	O2A-PA-O3	2.06	112.83	107.27
3	A	477	LMR	C2-C3-C4	2.04	117.42	112.08
2	B	476	NDP	O2N-PN-O1N	2.01	121.81	112.44
5	A	479	GOL	O1-C1-C2	2.01	119.43	110.38
2	B	476	NDP	O4B-C1B-C2B	-2.01	103.13	106.59

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	476	NDP	C5D-O5D-PN-O3
2	B	476	NDP	C5D-O5D-PN-O2N
3	A	477	LMR	O1A-C1-C2-O2
3	A	477	LMR	O2-C2-C3-C4
4	B	478	MLT	O1-C1-C2-O3
4	B	478	MLT	O2-C1-C2-O3
5	A	479	GOL	O1-C1-C2-C3
5	A	479	GOL	C1-C2-C3-O3
5	A	479	GOL	O2-C2-C3-O3
3	A	477	LMR	C1-C2-C3-C4
2	A	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	O4D-C1D-N1N-C6N
5	A	479	GOL	O1-C1-C2-O2
3	A	477	LMR	O1B-C1-C2-O2
4	B	477	MLT	O1-C1-C2-O3
4	B	477	MLT	O2-C1-C2-O3
2	A	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	PA-O3-PN-O2N
2	B	476	NDP	C2N-C3N-C7N-N7N
4	A	478	MLT	O2-C1-C2-O3
4	A	478	MLT	O2-C1-C2-C3
4	B	477	MLT	O1-C1-C2-C3
2	A	476	NDP	PA-O3-PN-O2N
2	B	476	NDP	C3B-C2B-O2B-P2B
4	A	478	MLT	O1-C1-C2-O3

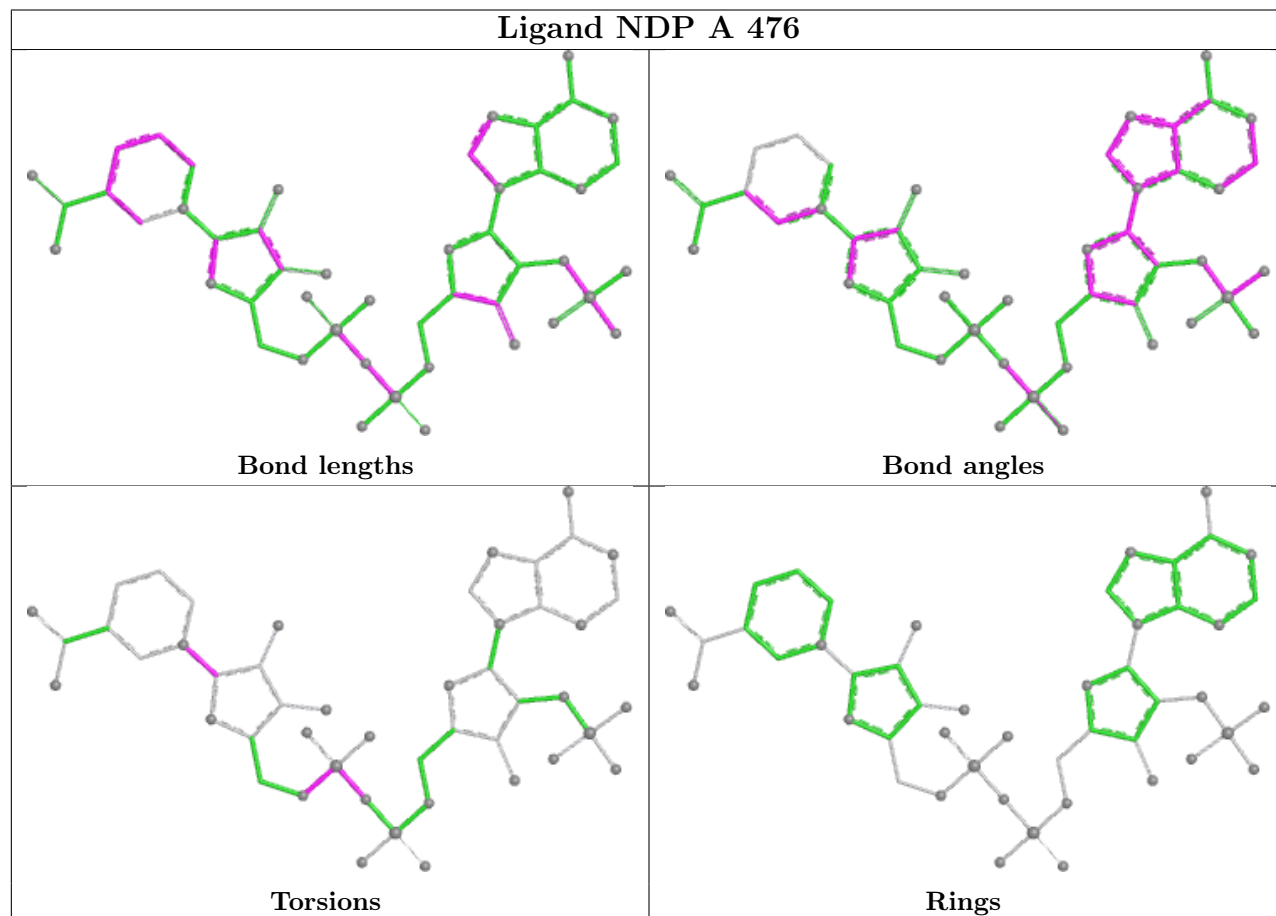
There are no ring outliers.

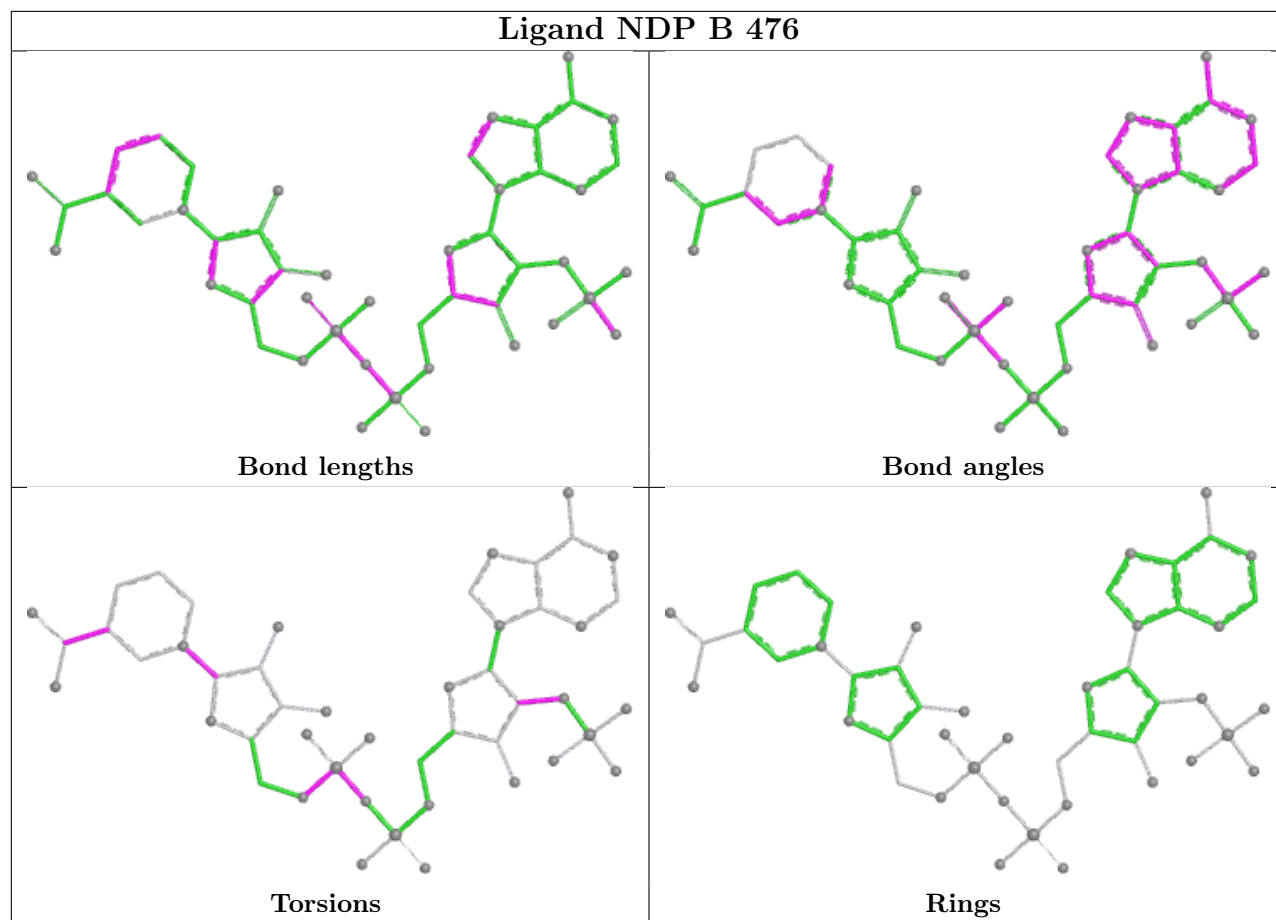
6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	479	GOL	6	0
2	A	476	NDP	1	0
4	B	478	MLT	5	0
2	B	476	NDP	1	0
5	B	479	GOL	2	0
4	A	478	MLT	4	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	476/496 (95%)	0.46	38 (7%) 18 18	8, 15, 35, 58	0
1	B	475/496 (95%)	0.47	40 (8%) 17 17	8, 15, 35, 59	0
All	All	951/992 (95%)	0.46	78 (8%) 17 17	8, 15, 35, 59	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	9.1
1	B	212	GLY	7.9
1	A	210	GLY	7.5
1	B	209	PRO	7.5
1	B	213	LYS	6.6
1	A	209	PRO	6.4
1	A	212	GLY	6.3
1	B	208	VAL	5.9
1	A	208	VAL	5.8
1	B	211	SER	5.6
1	A	407	VAL	5.4
1	A	211	SER	4.8
1	A	213	LYS	4.6
1	B	411	LEU	4.3
1	B	407	VAL	4.2
1	B	19	ARG	4.1
1	A	411	LEU	4.1
1	B	412	VAL	4.0
1	B	74	GLY	3.7
1	A	295	GLU	3.6
1	A	405	PRO	3.3
1	B	405	PRO	3.3
1	A	403	THR	3.3
1	A	412	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	410	ARG	3.1
1	B	410	ARG	3.1
1	B	413	ARG	3.0
1	A	294	PRO	3.0
1	B	72	ASP	3.0
1	A	166	GLU	3.0
1	A	406	GLU	2.9
1	B	402	ALA	2.9
1	B	70	ARG	2.9
1	B	166	GLU	2.9
1	B	342	ALA	2.9
1	B	73	GLU	2.9
1	B	406	GLU	2.9
1	B	55	LYS	2.9
1	A	72	ASP	2.8
1	B	48	ASP	2.8
1	B	-1	HIS	2.8
1	A	19	ARG	2.8
1	B	295	GLU	2.8
1	A	413	ARG	2.8
1	A	402	ALA	2.7
1	A	11	ARG	2.7
1	B	409	ASP	2.6
1	A	131	ARG	2.6
1	A	171	ARG	2.6
1	A	-1	HIS	2.6
1	A	48	ASP	2.6
1	B	130	GLY	2.6
1	A	70	ARG	2.6
1	B	131	ARG	2.5
1	B	394	GLY	2.5
1	A	394	GLY	2.4
1	A	414	GLN	2.4
1	B	171	ARG	2.4
1	A	404	ASP	2.4
1	A	74	GLY	2.4
1	A	409	ASP	2.3
1	B	404	ASP	2.3
1	B	403	THR	2.3
1	B	472	LEU	2.3
1	B	21	ALA	2.2
1	B	257	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	6	HIS	2.2
1	A	73	GLU	2.2
1	B	434	ASN	2.2
1	A	284	GLU	2.2
1	B	448	MET	2.2
1	A	473	SER	2.1
1	A	342	ALA	2.1
1	B	143	LEU	2.1
1	A	268	GLN	2.0
1	B	414	GLN	2.0
1	A	143	LEU	2.0
1	A	296	ASP	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 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.

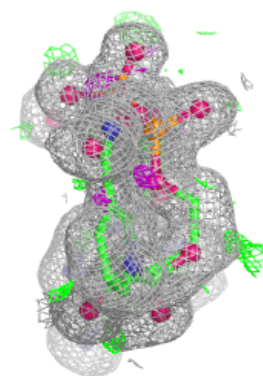
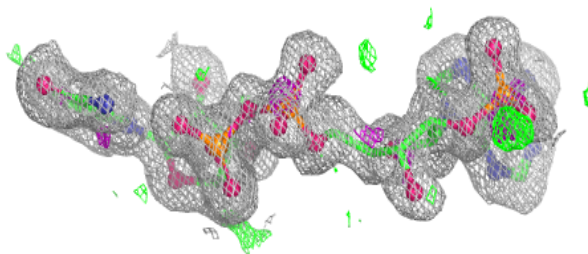
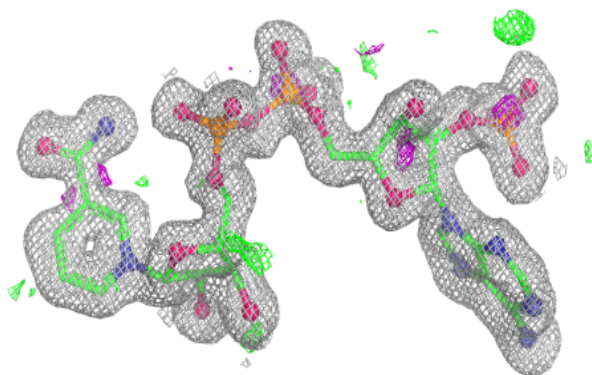
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMR	A	477	9/9	0.73	0.17	24,42,47,49	0
4	MLT	B	477	9/9	0.78	0.14	26,41,47,47	0
4	MLT	B	478	9/9	0.79	0.15	31,42,50,52	0
4	MLT	A	478	9/9	0.81	0.14	27,37,44,45	0
5	GOL	A	479	6/6	0.81	0.13	26,29,35,36	0
5	GOL	B	479	6/6	0.85	0.12	24,32,35,37	0
2	NDP	A	476	48/48	0.97	0.06	10,13,16,18	0
2	NDP	B	476	48/48	0.98	0.05	9,12,15,17	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.

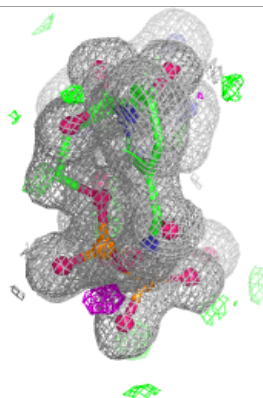
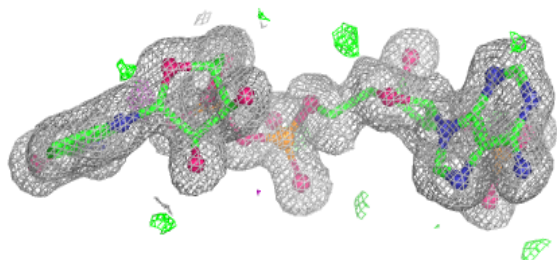
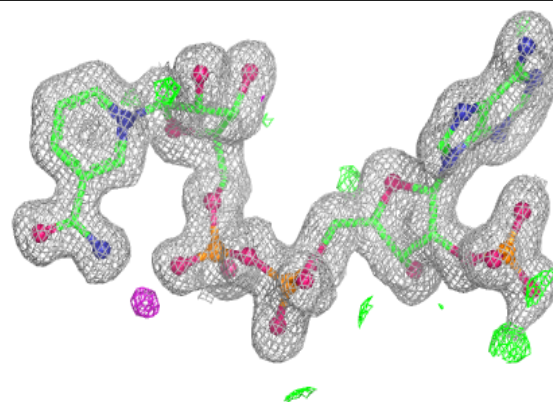
Electron density around NDP A 476:

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



Electron density around NDP B 476:

$2mF_o-DF_c$ (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.