



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 02:16 PM EDT

PDB ID : 3MJT
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 : 1.60 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 : 2.23.2
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) : 2.23.2

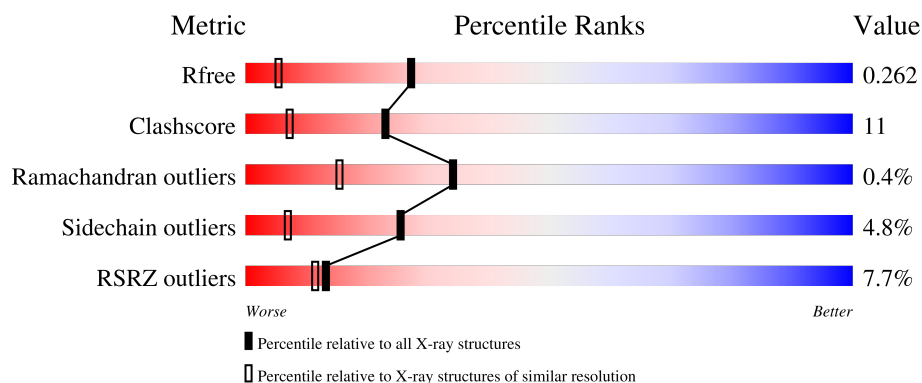
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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% 76% 17% . .
1	B	496	 7% 75% 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
2	NDP	A	476	X	-	-	-
2	NDP	B	476	X	-	-	-
3	GOL	A	477	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7581 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
			3466	2164	636	657	9			
1	B	475	Total	C	N	O	S	0	0	0
			3460	2161	635	655	9			

There are 44 discrepancies between the modelled and reference sequences:

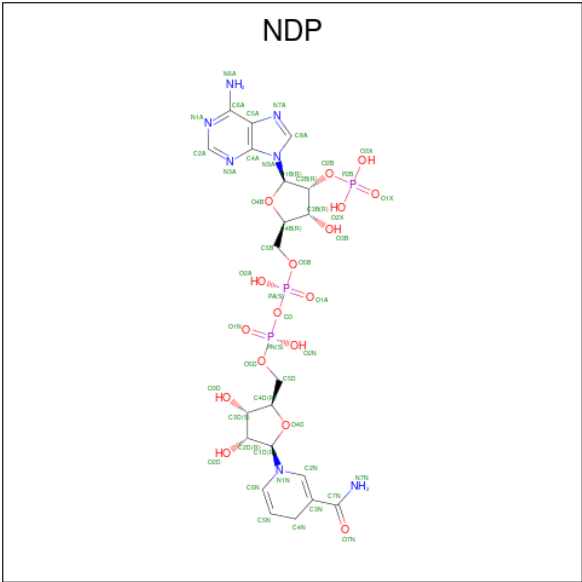
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q93NW7
A	-19	GLY	-	expression tag	UNP Q93NW7
A	-18	SER	-	expression tag	UNP Q93NW7
A	-17	SER	-	expression tag	UNP Q93NW7
A	-16	HIS	-	expression tag	UNP Q93NW7
A	-15	HIS	-	expression tag	UNP Q93NW7
A	-14	HIS	-	expression tag	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
A	364	HIS	GLN	engineered mutation	UNP Q93NW7
B	-20	MET	-	expression tag	UNP Q93NW7
B	-19	GLY	-	expression tag	UNP Q93NW7
B	-18	SER	-	expression tag	UNP Q93NW7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q93NW7
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
B	364	HIS	GLN	engineered mutation	UNP Q93NW7

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

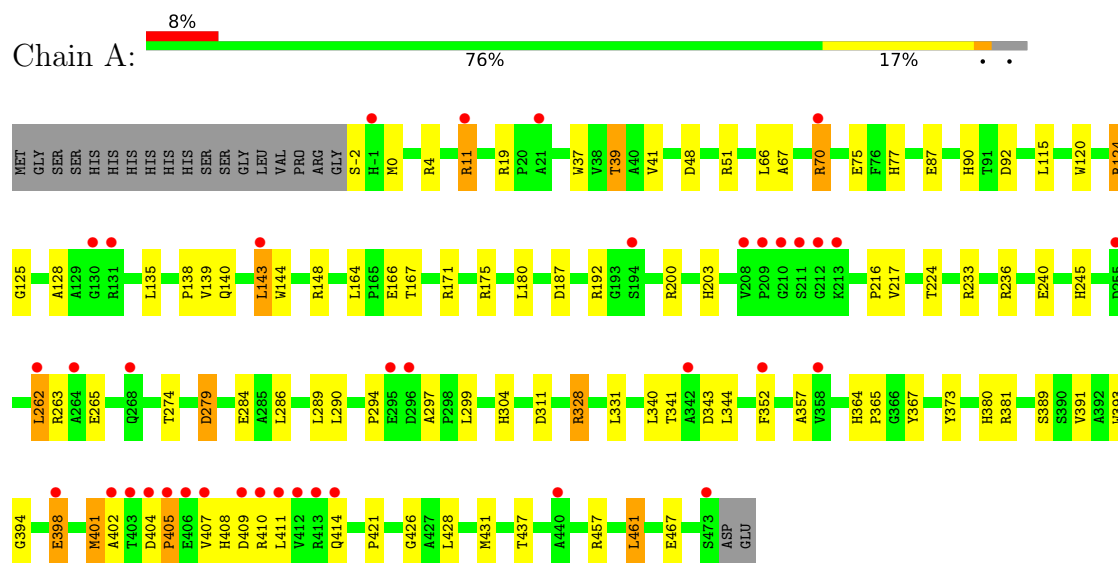
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	268	Total	O	0	0
			268	268		
4	B	279	Total	O	0	0
			279	279		

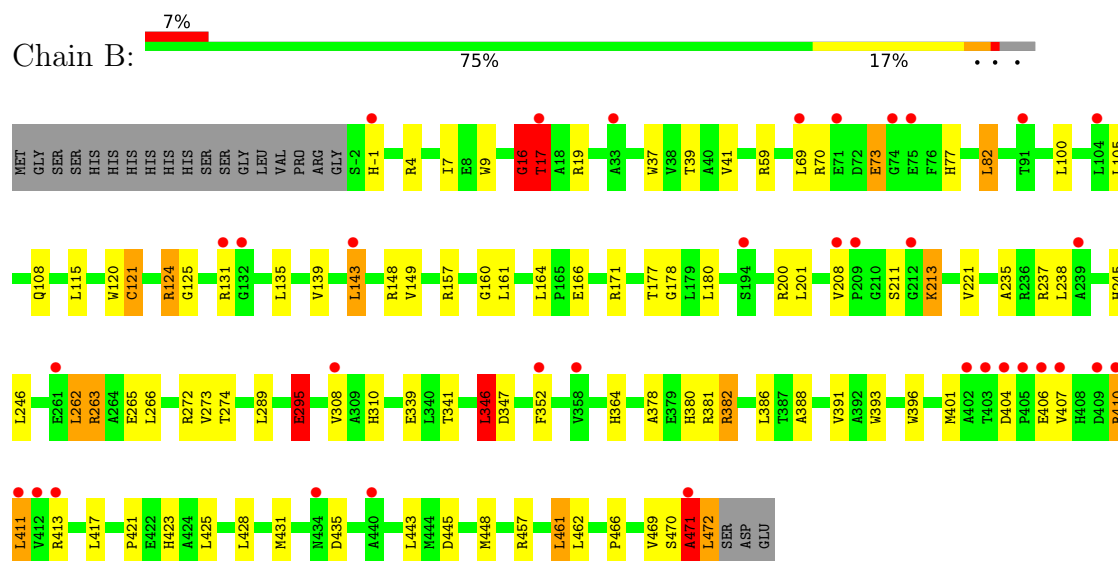
3 Residue-property plots [i](#)

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	61.40Å 63.61Å 71.85Å 72.84° 67.20° 89.77°	Depositor
Resolution (Å)	62.79 – 1.60 30.67 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.7 (62.79-1.60) 94.7 (30.67-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.223 , 0.265 0.222 , 0.262	Depositor DCC
R_{free} test set	5935 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.109 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NDP

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	1.26	5/3537 (0.1%)	1.19	21/4832 (0.4%)
1	B	1.27	8/3531 (0.2%)	1.32	32/4824 (0.7%)
All	All	1.27	13/7068 (0.2%)	1.25	53/9656 (0.5%)

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	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	TRP	CG-CD1	7.90	1.47	1.36
1	A	39	THR	CB-CG2	-7.00	1.29	1.52
1	B	457	ARG	CB-CG	-6.98	1.33	1.52
1	A	357	ALA	CA-CB	6.67	1.66	1.52
1	B	17	THR	N-CA	6.31	1.58	1.46
1	B	471	ALA	CA-CB	5.92	1.64	1.52
1	A	328	ARG	CG-CD	5.91	1.66	1.51
1	B	9	TRP	CZ3-CH2	5.83	1.49	1.40
1	A	120	TRP	CG-CD1	5.57	1.44	1.36
1	B	7	ILE	CB-CG2	5.43	1.69	1.52
1	B	295	GLU	CB-CG	5.42	1.62	1.52
1	B	139	VAL	CB-CG2	-5.33	1.41	1.52
1	A	144	TRP	CE3-CZ3	5.24	1.47	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	NE-CZ-NH1	25.26	132.93	120.30
1	B	382	ARG	NE-CZ-NH2	-21.11	109.74	120.30
1	B	121	CYS	CA-CB-SG	-13.34	89.99	114.00
1	A	200	ARG	NE-CZ-NH1	12.27	126.44	120.30
1	A	200	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	B	200	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	B	200	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	70	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	A	4	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	382	ARG	CD-NE-CZ	8.07	134.90	123.60
1	A	279	ASP	CB-CG-OD2	8.04	125.53	118.30
1	A	4	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	B	82	LEU	CB-CG-CD1	7.41	123.59	111.00
1	A	352	PHE	CB-CG-CD2	-7.35	115.65	120.80
1	B	381	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	B	263	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	48	ASP	CB-CG-OD1	7.04	124.63	118.30
1	B	148	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	B	4	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	472	LEU	CA-CB-CG	-6.72	99.83	115.30
1	B	17	THR	N-CA-C	6.70	129.09	111.00
1	B	115	LEU	CB-CG-CD1	6.39	121.86	111.00
1	A	51	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	192	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	148	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	401	MET	CG-SD-CE	6.27	110.23	100.20
1	B	346	LEU	CB-CG-CD2	6.21	121.56	111.00
1	B	289	LEU	CB-CG-CD2	-6.14	100.57	111.00
1	A	367	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	B	70	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	B	457	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	124	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	115	LEU	CB-CG-CD2	5.88	120.99	111.00
1	A	175	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	382	ARG	CB-CG-CD	5.82	126.73	111.60
1	B	4	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	157	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	B	272	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	B	386	LEU	CB-CG-CD1	5.74	120.75	111.00
1	B	381	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	289	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	B	346	LEU	CB-CG-CD1	5.64	120.59	111.00
1	A	192	ARG	NE-CZ-NH2	-5.59	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	352	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	B	401	MET	CG-SD-CE	5.43	108.89	100.20
1	B	16	GLY	C-N-CA	-5.33	108.38	121.70
1	B	347	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	143	LEU	CB-CG-CD2	-5.27	102.05	111.00
1	B	149	VAL	CA-CB-CG2	-5.11	103.24	110.90
1	A	461	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	381	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	187	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	16	GLY	Peptide
1	B	17	THR	Peptide
1	B	471	ALA	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	3466	0	3425	66	0
1	B	3460	0	3420	93	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
3	A	6	0	8	4	0
3	B	6	0	8	0	0
4	A	268	0	0	12	0
4	B	279	0	0	8	0
All	All	7581	0	6911	159	0

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

All (159) 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:121:CYS:HB3	4:B:756:HOH:O	1.11	1.27
1:B:121:CYS:SG	1:B:121:CYS:O	2.04	1.14
1:B:461:LEU:O	1:B:461:LEU:HD13	1.54	1.08
1:B:470:SER:O	1:B:471:ALA:HB3	1.55	1.03
1:B:121:CYS:SG	1:B:161:LEU:HD23	2.02	0.98
1:B:208:VAL:HG23	1:B:211:SER:OG	1.65	0.96
1:A:263:ARG:HD3	4:A:666:HOH:O	1.67	0.94
1:B:461:LEU:HD13	1:B:461:LEU:C	1.88	0.94
1:B:407:VAL:O	1:B:411:LEU:HD13	1.67	0.93
1:B:262:LEU:O	1:B:266:LEU:HD13	1.69	0.92
1:B:470:SER:O	1:B:471:ALA:CB	2.16	0.92
1:B:17:THR:HG21	1:B:177:THR:OG1	1.68	0.92
1:A:90:HIS:HD2	1:A:92:ASP:H	1.13	0.91
1:B:391:VAL:HG21	1:B:428:LEU:HD13	1.57	0.87
1:B:201:LEU:HB2	1:B:461:LEU:HD11	1.56	0.85
1:A:404:ASP:HB3	1:A:407:VAL:HG22	1.59	0.84
1:B:59:ARG:HB2	1:B:105:LEU:HD12	1.58	0.84
1:B:121:CYS:SG	1:B:161:LEU:HA	2.18	0.84
1:A:391:VAL:HG21	1:A:428:LEU:HD13	1.58	0.83
1:A:341:THR:HA	1:A:344:LEU:HD13	1.59	0.82
1:B:461:LEU:C	1:B:461:LEU:CD1	2.47	0.82
1:A:216:PRO:HA	3:A:477:GOL:H31	1.64	0.79
1:A:11:ARG:HH21	1:A:11:ARG:HG3	1.48	0.78
1:B:411:LEU:CD1	1:B:411:LEU:H	1.97	0.78
1:B:41:VAL:HG21	1:B:164:LEU:HD11	1.65	0.77
1:A:240:GLU:OE1	4:A:511:HOH:O	2.03	0.76
1:B:295:GLU:H	1:B:295:GLU:CD	1.89	0.75
1:B:59:ARG:HB2	1:B:105:LEU:CD1	2.17	0.75
1:A:224:THR:OG1	1:A:304:HIS:HD2	1.73	0.71
1:A:39:THR:HB	4:A:731:HOH:O	1.90	0.71
1:B:41:VAL:CG2	1:B:164:LEU:HD11	2.19	0.71
1:B:407:VAL:O	1:B:411:LEU:CD1	2.39	0.71
1:A:217:VAL:H	3:A:477:GOL:H11	1.57	0.69
1:B:471:ALA:O	1:B:472:LEU:C	2.31	0.69
1:B:39:THR:HB	4:B:500:HOH:O	1.92	0.68
1:B:201:LEU:CB	1:B:461:LEU:HD11	2.21	0.68
1:A:263:ARG:NH2	4:A:666:HOH:O	2.06	0.67
1:A:203:HIS:HE1	1:A:467:GLU:OE2	1.76	0.67
1:A:263:ARG:CD	4:A:666:HOH:O	2.35	0.65
1:A:411:LEU:O	1:A:414:GLN:HG2	1.95	0.65
1:B:37:TRP:CE3	1:B:164:LEU:HD12	2.31	0.65
1:B:461:LEU:HD12	1:B:462:LEU:HD23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HH21	1:A:11:ARG:CG	2.09	0.64
1:B:466:PRO:O	1:B:469:VAL:CG2	2.45	0.64
1:A:398:GLU:HG3	1:A:421:PRO:CD	2.28	0.64
1:B:121:CYS:SG	1:B:161:LEU:CD2	2.81	0.63
1:A:77:HIS:HE1	1:A:180:LEU:O	1.81	0.63
1:B:208:VAL:HG23	1:B:211:SER:HG	1.63	0.63
1:A:203:HIS:HD2	4:A:512:HOH:O	1.81	0.63
1:A:284:GLU:HB2	4:A:671:HOH:O	1.99	0.63
1:A:286:LEU:HD23	1:A:340:LEU:HD12	1.80	0.62
1:B:100:LEU:HD12	1:B:143:LEU:HD13	1.81	0.62
1:A:166:GLU:H	1:A:166:GLU:CD	2.03	0.62
1:A:135:LEU:O	1:A:380:HIS:HD2	1.83	0.61
1:B:411:LEU:HD13	1:B:411:LEU:H	1.65	0.61
1:A:402:ALA:O	1:A:408:HIS:HB2	2.01	0.61
1:B:393:TRP:HB2	2:B:476:NDP:C5N	2.31	0.61
1:A:245:HIS:HE1	1:A:274:THR:OG1	1.83	0.60
1:A:224:THR:OG1	1:A:304:HIS:CD2	2.53	0.60
1:B:466:PRO:HA	1:B:469:VAL:CG2	2.31	0.60
1:B:17:THR:CG2	1:B:177:THR:OG1	2.47	0.59
1:A:414:GLN:NE2	4:A:591:HOH:O	2.35	0.59
1:B:411:LEU:CD1	1:B:411:LEU:N	2.64	0.59
1:B:364:HIS:HD2	4:B:550:HOH:O	1.86	0.58
1:A:391:VAL:HG22	1:A:431:MET:SD	2.44	0.58
1:B:245:HIS:HE1	1:B:274:THR:OG1	1.85	0.58
1:A:67:ALA:O	1:A:70:ARG:HG3	2.03	0.58
1:A:90:HIS:CD2	1:A:92:ASP:H	2.06	0.56
1:B:411:LEU:N	1:B:411:LEU:HD12	2.20	0.56
1:B:466:PRO:O	1:B:469:VAL:HG22	2.05	0.56
1:B:17:THR:HG23	1:B:178:GLY:N	2.21	0.56
1:B:266:LEU:HD12	1:B:266:LEU:N	2.20	0.55
1:B:391:VAL:HG22	1:B:431:MET:SD	2.47	0.55
1:B:77:HIS:HE1	1:B:180:LEU:O	1.90	0.55
1:B:105:LEU:HD13	1:B:108:GLN:OE1	2.06	0.55
1:A:391:VAL:HG21	1:A:428:LEU:CD1	2.34	0.55
1:B:171:ARG:NH1	4:B:484:HOH:O	2.39	0.54
1:B:266:LEU:N	1:B:266:LEU:CD1	2.70	0.54
1:B:471:ALA:O	1:B:472:LEU:O	2.25	0.54
1:B:413:ARG:O	1:B:448:MET:HE2	2.07	0.54
1:A:279:ASP:OD1	1:A:328:ARG:NH2	2.41	0.54
1:B:308:VAL:HG13	1:B:310:HIS:ND1	2.23	0.54
1:A:37:TRP:CG	1:A:124:ARG:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:PRO:O	1:B:469:VAL:HG23	2.07	0.53
1:B:466:PRO:HA	1:B:469:VAL:HG22	1.89	0.53
1:A:405:PRO:HA	1:A:409:ASP:OD1	2.08	0.53
1:A:70:ARG:HG2	1:A:115:LEU:HD11	1.91	0.52
1:A:401:MET:O	1:A:407:VAL:HG21	2.10	0.52
1:B:262:LEU:HD22	1:B:266:LEU:HD11	1.92	0.52
1:B:16:GLY:O	1:B:17:THR:C	2.47	0.52
1:B:263:ARG:HG3	1:B:273:VAL:HG11	1.92	0.52
1:B:382:ARG:HD3	1:B:388:ALA:O	2.09	0.52
1:B:19:ARG:CZ	1:B:19:ARG:HB3	2.41	0.51
1:B:391:VAL:HG21	1:B:428:LEU:CD1	2.35	0.51
1:B:341:THR:HB	1:B:346:LEU:HD22	1.92	0.51
1:A:410:ARG:HG3	1:A:411:LEU:H	1.75	0.51
1:B:221:VAL:HG11	1:B:238:LEU:HD13	1.91	0.51
1:A:236:ARG:CD	4:A:523:HOH:O	2.58	0.50
1:A:398:GLU:HG3	1:A:421:PRO:HD3	1.94	0.50
1:A:217:VAL:H	3:A:477:GOL:C1	2.22	0.50
1:B:39:THR:CB	4:B:500:HOH:O	2.56	0.50
1:A:66:LEU:O	1:A:70:ARG:HG2	2.12	0.50
1:B:308:VAL:CG1	1:B:310:HIS:CE1	2.95	0.50
1:B:417:LEU:HB2	1:B:443:LEU:HD23	1.95	0.49
1:B:69:LEU:O	1:B:73:GLU:HG2	2.12	0.49
1:B:235:ALA:HB1	1:B:246:LEU:HD13	1.93	0.49
1:A:124:ARG:H	1:A:140:GLN:NE2	2.10	0.49
1:A:404:ASP:CB	1:A:407:VAL:HG22	2.36	0.49
1:B:135:LEU:O	1:B:380:HIS:HD2	1.95	0.49
1:A:236:ARG:HD2	1:A:265:GLU:OE1	2.12	0.49
1:B:378:ALA:O	1:B:382:ARG:HG2	2.12	0.49
1:B:41:VAL:CG2	1:B:164:LEU:CD1	2.90	0.48
1:A:216:PRO:HA	3:A:477:GOL:H11	1.97	0.47
1:B:100:LEU:CD1	1:B:143:LEU:HD13	2.45	0.47
1:B:213:LYS:HD2	1:B:435:ASP:HB2	1.96	0.47
1:A:286:LEU:CD2	1:A:340:LEU:HD12	2.45	0.46
1:B:341:THR:HB	1:B:346:LEU:CD2	2.45	0.46
1:A:404:ASP:HB3	1:A:407:VAL:CG2	2.39	0.46
1:B:237:ARG:CD	1:B:425:LEU:HD13	2.46	0.46
1:A:39:THR:CB	4:A:731:HOH:O	2.55	0.46
1:A:138:PRO:HB2	1:A:373:TYR:CE1	2.50	0.46
1:B:37:TRP:HE3	1:B:164:LEU:HD12	1.81	0.46
1:B:262:LEU:HD22	1:B:266:LEU:CD1	2.46	0.46
1:B:308:VAL:HG13	1:B:310:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:HD3	4:A:523:HOH:O	2.16	0.46
1:A:294:PRO:HG2	1:A:297:ALA:HB3	1.98	0.45
1:A:393:TRP:HB2	2:A:476:NDP:C5N	2.46	0.45
1:A:389:SER:HA	1:A:437:THR:O	2.15	0.45
1:A:125:GLY:HA2	4:A:552:HOH:O	2.16	0.45
1:A:124:ARG:H	1:A:140:GLN:HE22	1.63	0.44
1:B:41:VAL:HG21	1:B:164:LEU:CD1	2.41	0.44
1:B:396:TRP:HH2	1:B:425:LEU:HD21	1.83	0.44
1:B:143:LEU:HD13	1:B:143:LEU:HA	1.89	0.43
1:B:121:CYS:SG	1:B:160:GLY:O	2.75	0.43
1:B:339:GLU:OE1	4:B:497:HOH:O	2.22	0.43
1:A:41:VAL:HG21	1:A:164:LEU:HD11	2.01	0.43
1:A:135:LEU:O	1:A:380:HIS:CD2	2.68	0.42
1:A:233:ARG:HD2	1:A:233:ARG:HA	1.84	0.42
1:B:125:GLY:HA2	4:B:551:HOH:O	2.20	0.42
1:B:201:LEU:CB	1:B:461:LEU:CD1	2.95	0.42
1:A:398:GLU:HG3	1:A:421:PRO:HD2	2.02	0.42
1:A:290:LEU:HD22	1:A:299:LEU:HD22	2.01	0.42
1:B:466:PRO:CA	1:B:469:VAL:HG22	2.50	0.42
1:A:128:ALA:HB2	1:A:135:LEU:HB2	2.02	0.41
1:B:308:VAL:HG11	1:B:310:HIS:CE1	2.54	0.41
1:B:105:LEU:HD13	1:B:105:LEU:HA	1.82	0.41
1:B:406:GLU:O	1:B:410:ARG:HG2	2.19	0.41
1:B:59:ARG:CB	1:B:105:LEU:HD12	2.40	0.41
1:B:213:LYS:HD2	4:B:542:HOH:O	2.21	0.41
1:A:341:THR:CA	1:A:344:LEU:HD13	2.40	0.41
1:B:266:LEU:CD1	1:B:266:LEU:H	2.33	0.41
1:B:404:ASP:C	1:B:406:GLU:H	2.23	0.41
1:B:469:VAL:HG23	1:B:470:SER:N	2.36	0.41
1:A:87:GLU:HB3	1:A:139:VAL:HG21	2.03	0.40
1:A:364:HIS:N	1:A:365:PRO:CD	2.85	0.40
1:B:208:VAL:CG2	1:B:211:SER:OG	2.53	0.40
1:A:0:MET:SD	1:A:426:GLY:HA3	2.61	0.40
1:A:331:LEU:HA	1:A:373:TYR:CD2	2.55	0.40
1:B:417:LEU:HD11	1:B:445:ASP:HB2	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	474/496 (96%)	459 (97%)	13 (3%)	2 (0%)	34	15
1	B	473/496 (95%)	459 (97%)	12 (2%)	2 (0%)	34	15
All	All	947/992 (96%)	918 (97%)	25 (3%)	4 (0%)	34	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	471	ALA
1	A	394	GLY
1	A	405	PRO

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	334/351 (95%)	320 (96%)	14 (4%)	30	9
1	B	333/351 (95%)	315 (95%)	18 (5%)	22	5
All	All	667/702 (95%)	635 (95%)	32 (5%)	25	7

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	11	ARG

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Mol	Chain	Res	Type
1	A	19	ARG
1	A	75	GLU
1	A	124	ARG
1	A	143	LEU
1	A	167	THR
1	A	171	ARG
1	A	262	LEU
1	A	311	ASP
1	A	343	ASP
1	A	398	GLU
1	A	457	ARG
1	A	461	LEU
1	B	-1	HIS
1	B	17	THR
1	B	73	GLU
1	B	82	LEU
1	B	124	ARG
1	B	131	ARG
1	B	143	LEU
1	B	166	GLU
1	B	213	LYS
1	B	262	LEU
1	B	265	GLU
1	B	295	GLU
1	B	346	LEU
1	B	410	ARG
1	B	411	LEU
1	B	421	PRO
1	B	423	HIS
1	B	461	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	77	HIS
1	A	90	HIS
1	A	102	GLN
1	A	140	GLN
1	A	203	HIS
1	A	245	HIS
1	A	304	HIS

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Mol	Chain	Res	Type
1	A	310	HIS
1	A	336	HIS
1	A	380	HIS
1	A	414	GLN
1	A	456	ASN
1	B	32	HIS
1	B	77	HIS
1	B	102	GLN
1	B	241	GLN
1	B	245	HIS
1	B	336	HIS
1	B	364	HIS
1	B	380	HIS
1	B	408	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	GOL	A	477	-	5,5,5	0.49	0	5,5,5	0.47	0
2	NDP	B	476	-	45,52,52	1.64	9 (20%)	53,80,80	2.11	17 (32%)
3	GOL	B	477	-	5,5,5	0.56	0	5,5,5	0.81	0
2	NDP	A	476	-	45,52,52	1.50	8 (17%)	53,80,80	2.09	14 (26%)

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	GOL	A	477	-	-	4/4/4/4	-
2	NDP	B	476	-	1/1/14/17	8/30/77/77	0/5/5/5
3	GOL	B	477	-	-	0/4/4/4	-
2	NDP	A	476	-	1/1/14/17	6/30/77/77	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	476	NDP	C4N-C3N	-4.99	1.40	1.49
2	A	476	NDP	C4N-C3N	-4.98	1.40	1.49
2	B	476	NDP	O4B-C1B	3.96	1.46	1.41
2	B	476	NDP	C4N-C5N	-3.59	1.39	1.48
2	B	476	NDP	O4D-C1D	3.48	1.50	1.42
2	A	476	NDP	C4N-C5N	-3.12	1.40	1.48
2	B	476	NDP	C8A-N7A	2.80	1.39	1.34
2	B	476	NDP	C6N-C5N	2.77	1.38	1.33
2	A	476	NDP	C6N-C5N	2.76	1.38	1.33
2	A	476	NDP	C5A-C4A	-2.49	1.34	1.40
2	B	476	NDP	C1D-N1N	2.39	1.53	1.46
2	B	476	NDP	C5A-N7A	-2.19	1.31	1.39
2	A	476	NDP	C4A-N3A	2.17	1.38	1.35
2	A	476	NDP	O4B-C1B	2.15	1.44	1.41
2	A	476	NDP	O3B-C3B	2.09	1.47	1.43
2	B	476	NDP	O5B-C5B	-2.04	1.36	1.44
2	A	476	NDP	C2D-C3D	-2.04	1.47	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	N3A-C2A-N1A	-6.84	117.98	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	476	NDP	O4B-C4B-C3B	6.28	117.55	105.11
2	B	476	NDP	N3A-C2A-N1A	-5.91	119.44	128.68
2	A	476	NDP	C2B-C3B-C4B	-5.38	90.31	101.99
2	B	476	NDP	O4B-C4B-C3B	4.91	114.83	105.11
2	B	476	NDP	C2B-C3B-C4B	-4.89	91.38	101.99
2	B	476	NDP	C2A-N1A-C6A	4.60	126.62	118.75
2	B	476	NDP	C5B-C4B-C3B	3.29	127.52	115.18
2	B	476	NDP	C5A-C6A-N6A	3.26	125.31	120.35
2	B	476	NDP	O7N-C7N-C3N	-3.22	114.83	120.90
2	A	476	NDP	O4B-C4B-C5B	3.17	119.81	109.37
2	B	476	NDP	O2B-P2B-O1X	-3.16	97.18	109.39
2	A	476	NDP	C2A-N1A-C6A	3.04	123.95	118.75
2	A	476	NDP	O7N-C7N-C3N	-2.98	115.28	120.90
2	A	476	NDP	O2B-P2B-O1X	-2.89	98.25	109.39
2	B	476	NDP	C5A-C6A-N1A	-2.86	113.86	120.35
2	A	476	NDP	C3N-C2N-N1N	-2.77	119.14	123.10
2	B	476	NDP	O2B-C2B-C1B	2.64	119.60	110.10
2	B	476	NDP	C3N-C2N-N1N	-2.63	119.35	123.10
2	B	476	NDP	O4B-C4B-C5B	2.50	117.61	109.37
2	B	476	NDP	C2D-C3D-C4D	2.50	107.50	102.64
2	A	476	NDP	O3X-P2B-O2X	2.21	116.09	107.64
2	B	476	NDP	O3D-C3D-C2D	-2.19	104.75	111.82
2	A	476	NDP	O4D-C1D-C2D	-2.18	101.88	106.64
2	A	476	NDP	O2D-C2D-C3D	2.17	118.84	111.82
2	B	476	NDP	C1B-N9A-C4A	-2.15	122.87	126.64
2	A	476	NDP	C1B-N9A-C4A	-2.12	122.92	126.64
2	A	476	NDP	C4D-O4D-C1D	2.05	113.99	109.47
2	A	476	NDP	C2D-C3D-C4D	2.04	106.60	102.64
2	B	476	NDP	O3X-P2B-O2X	2.04	115.42	107.64
2	B	476	NDP	O2D-C2D-C3D	2.03	118.38	111.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	476	NDP	C4B
2	B	476	NDP	C4B

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	476	NDP	C5D-O5D-PN-O1N
2	A	476	NDP	C5D-O5D-PN-O2N

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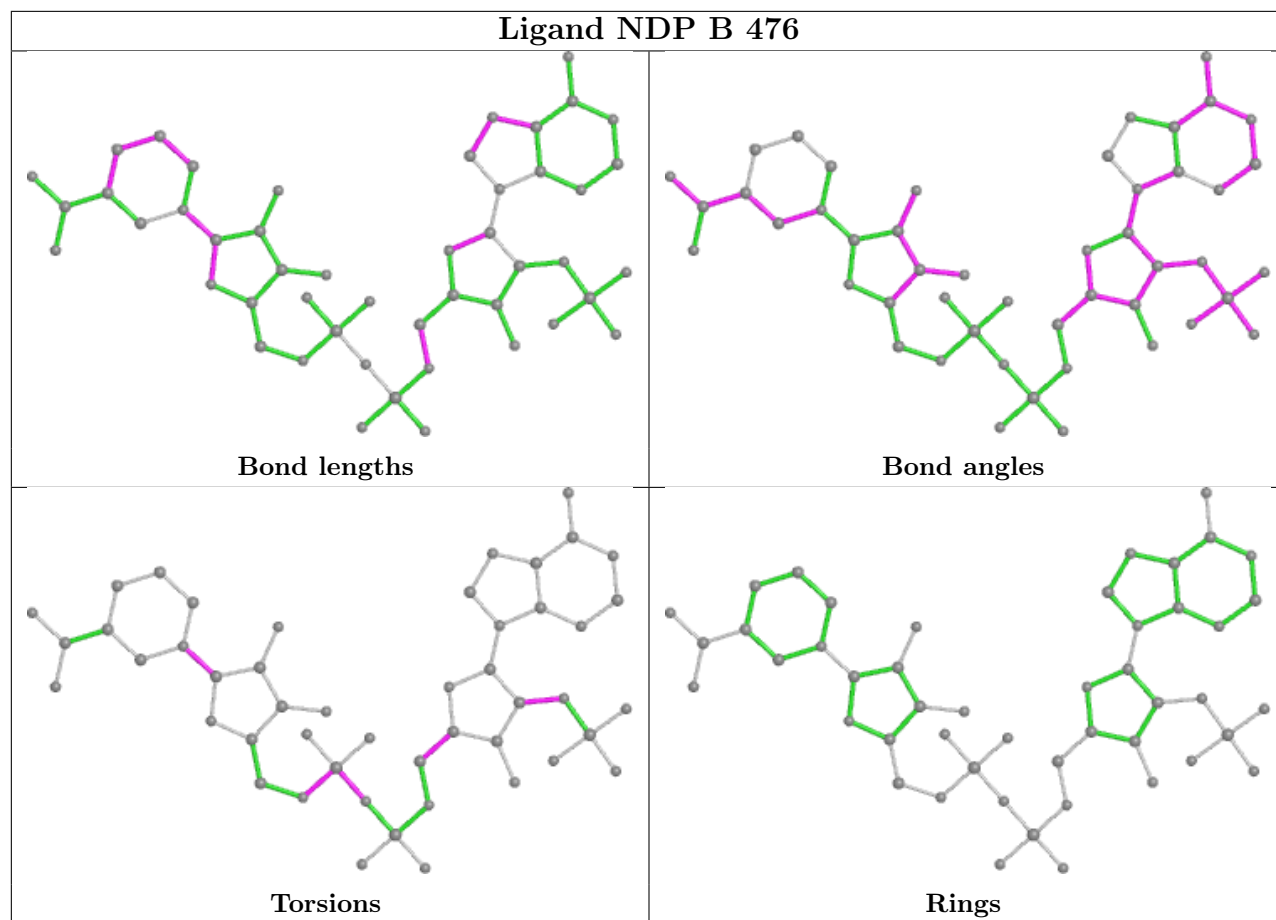
Mol	Chain	Res	Type	Atoms
2	B	476	NDP	C5D-O5D-PN-O1N
2	B	476	NDP	C5D-O5D-PN-O2N
3	A	477	GOL	O1-C1-C2-C3
3	A	477	GOL	C1-C2-C3-O3
2	A	476	NDP	O4B-C4B-C5B-O5B
2	B	476	NDP	O4B-C4B-C5B-O5B
3	A	477	GOL	O2-C2-C3-O3
3	A	477	GOL	O1-C1-C2-O2
2	B	476	NDP	C3B-C4B-C5B-O5B
2	A	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	O4D-C1D-N1N-C6N
2	B	476	NDP	C1B-C2B-O2B-P2B
2	A	476	NDP	C5D-O5D-PN-O3
2	B	476	NDP	C5D-O5D-PN-O3
2	A	476	NDP	PA-O3-PN-O1N
2	B	476	NDP	PA-O3-PN-O2N

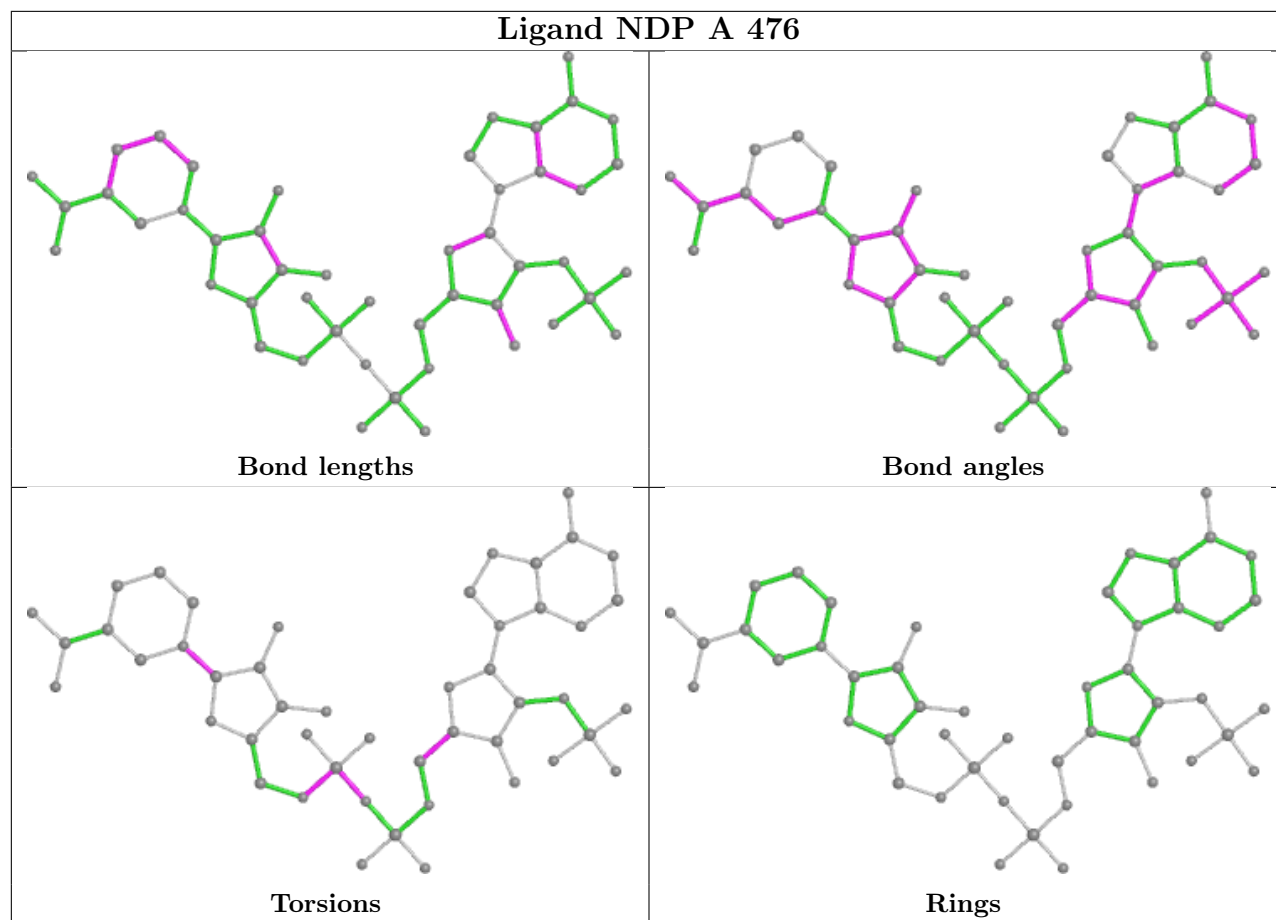
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	477	GOL	4	0
2	B	476	NDP	1	0
2	A	476	NDP	1	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%)	0.64	38 (7%) 12 11	9, 17, 34, 60	0
1	B	475/496 (95%)	0.54	35 (7%) 14 13	8, 16, 34, 61	0
All	All	951/992 (95%)	0.59	73 (7%) 13 11	8, 17, 34, 61	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	LEU	8.7
1	B	402	ALA	7.7
1	B	405	PRO	6.9
1	B	471	ALA	6.7
1	A	412	VAL	6.2
1	A	407	VAL	6.1
1	A	413	ARG	6.0
1	A	402	ALA	5.8
1	B	17	THR	5.2
1	A	208	VAL	5.1
1	A	405	PRO	5.1
1	B	413	ARG	4.9
1	A	410	ARG	4.9
1	A	-1	HIS	4.8
1	A	131	ARG	4.6
1	A	21	ALA	4.2
1	B	131	ARG	4.2
1	A	406	GLU	4.1
1	A	209	PRO	3.9
1	B	406	GLU	3.8
1	B	411	LEU	3.8
1	B	-1	HIS	3.7
1	A	211	SER	3.7
1	B	143	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	3.6
1	A	358	VAL	3.5
1	B	407	VAL	3.4
1	A	210	GLY	3.4
1	B	410	ARG	3.2
1	A	404	ASP	3.1
1	A	409	ASP	3.1
1	A	352	PHE	3.0
1	B	404	ASP	3.0
1	B	412	VAL	2.9
1	B	71	GLU	2.9
1	A	213	LYS	2.9
1	A	295	GLU	2.8
1	A	143	LEU	2.8
1	A	11	ARG	2.7
1	A	342	ALA	2.7
1	B	208	VAL	2.7
1	A	70	ARG	2.6
1	A	440	ALA	2.5
1	B	358	VAL	2.5
1	B	409	ASP	2.4
1	B	74	GLY	2.4
1	A	403	THR	2.4
1	A	255	ASP	2.4
1	B	91	THR	2.4
1	B	403	THR	2.4
1	A	268	GLN	2.4
1	A	398	GLU	2.3
1	A	414	GLN	2.3
1	B	194	SER	2.3
1	B	261	GLU	2.2
1	B	434	ASN	2.2
1	B	75	GLU	2.2
1	A	473	SER	2.2
1	A	130	GLY	2.2
1	B	132	GLY	2.2
1	B	440	ALA	2.1
1	A	262	LEU	2.1
1	A	264	ALA	2.1
1	B	33	ALA	2.1
1	B	69	LEU	2.1
1	B	104	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	194	SER	2.1
1	B	212	GLY	2.1
1	B	209	PRO	2.0
1	B	352	PHE	2.0
1	B	239	ALA	2.0
1	B	308	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

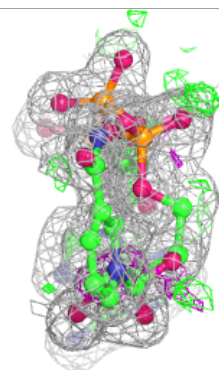
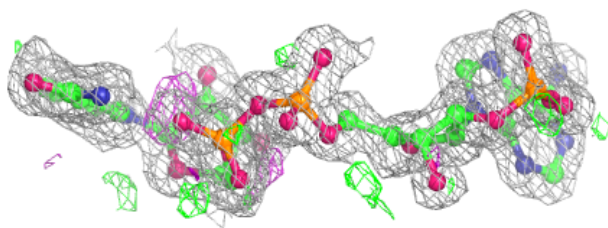
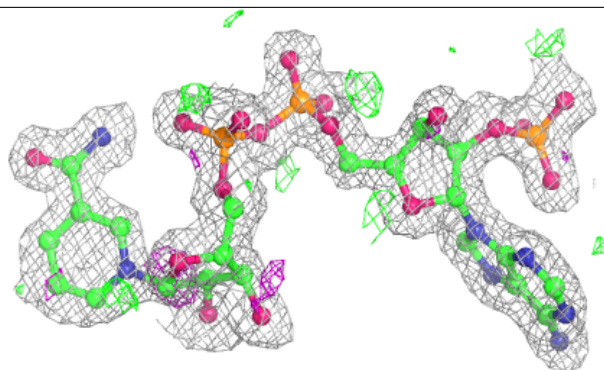
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	477	6/6	0.81	0.14	32,33,38,40	0
3	GOL	B	477	6/6	0.88	0.12	23,24,28,29	0
2	NDP	A	476	48/48	0.94	0.11	12,18,22,22	0
2	NDP	B	476	48/48	0.95	0.10	11,15,19,20	0

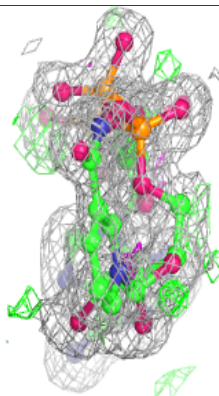
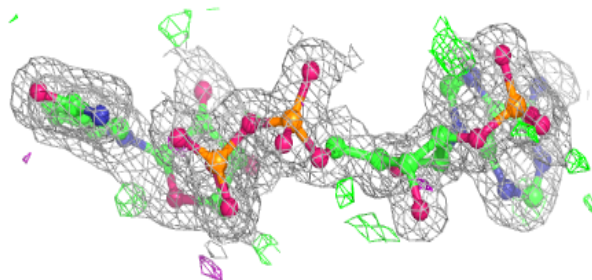
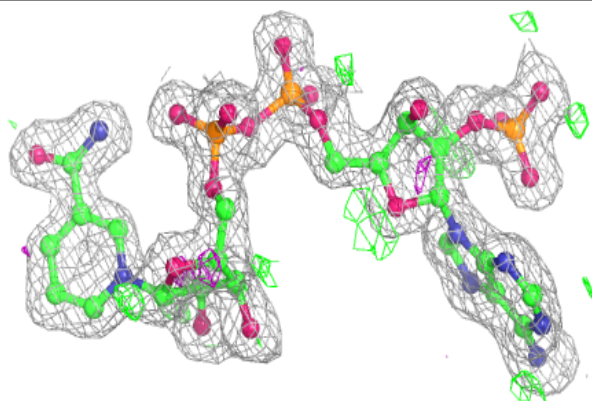
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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.