Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2024 – 04:58 pm BST

PDB ID	:	8S65
Title	:	1-deoxy-D-xylulose 5-phosphate reductoisomerase (DXR) as target for anti Toxoplasma gondii compounds: crystal structure, biochemical characterization and biological evaluation of inhibitors
Authors	:	Mazzone, F.; Hoeppner, A.; Reiners, J.; Applegate, V.; Abdullaziz, M.; Gottstein, J.; Wesemann, M.; Kurz, T.; Smits, S.H.; Pfeffer, K.
Deposited on	:	2024-02-26
Resolution	:	2.56 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 (i) 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 (1)) were used in the production of this report:

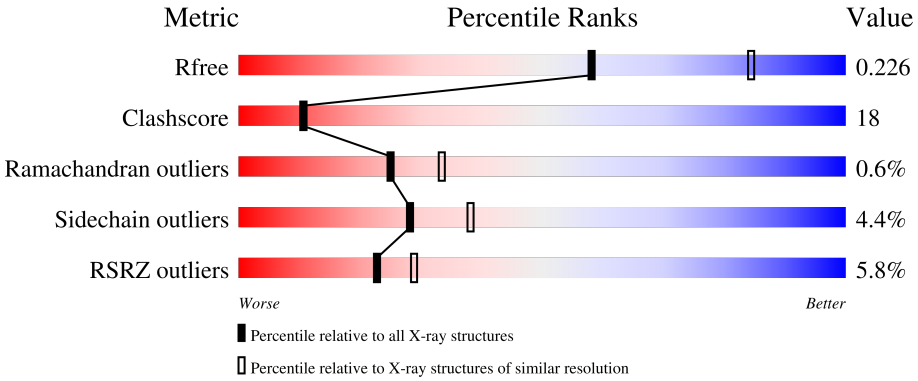
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION, SOLUTION SCATTERING

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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 <=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	472	2% 62% 22% • • 13%
1	B	472	8% 57% 26% • • 13%

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	FOM	A	502	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12821 atoms, of which 6405 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 1-deoxy-D-xylulose-5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	H	N	O	S	0	0	0
			6292	1989	3159	554	579	11			
1	B	411	Total	C	H	N	O	S	0	1	0
			6330	1999	3180	559	581	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP S8ESX0
A	2	GLY	-	expression tag	UNP S8ESX0
A	3	HIS	-	expression tag	UNP S8ESX0
A	4	HIS	-	expression tag	UNP S8ESX0
A	5	HIS	-	expression tag	UNP S8ESX0
A	6	HIS	-	expression tag	UNP S8ESX0
A	7	HIS	-	expression tag	UNP S8ESX0
A	8	HIS	-	expression tag	UNP S8ESX0
A	9	HIS	-	expression tag	UNP S8ESX0
A	10	HIS	-	expression tag	UNP S8ESX0
A	11	HIS	-	expression tag	UNP S8ESX0
A	12	HIS	-	expression tag	UNP S8ESX0
A	13	SER	-	expression tag	UNP S8ESX0
A	14	SER	-	expression tag	UNP S8ESX0
A	15	GLY	-	expression tag	UNP S8ESX0
A	16	HIS	-	expression tag	UNP S8ESX0
A	17	ILE	-	expression tag	UNP S8ESX0
A	18	GLU	-	expression tag	UNP S8ESX0
A	19	GLY	-	expression tag	UNP S8ESX0
A	20	ARG	-	expression tag	UNP S8ESX0
A	21	HIS	-	expression tag	UNP S8ESX0
A	22	MET	-	expression tag	UNP S8ESX0
B	1	MET	-	initiating methionine	UNP S8ESX0
B	2	GLY	-	expression tag	UNP S8ESX0
B	3	HIS	-	expression tag	UNP S8ESX0

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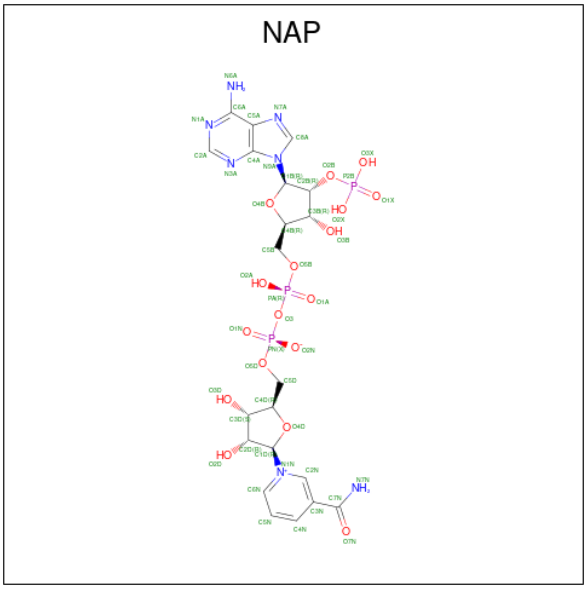
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP S8ESX0
B	5	HIS	-	expression tag	UNP S8ESX0
B	6	HIS	-	expression tag	UNP S8ESX0
B	7	HIS	-	expression tag	UNP S8ESX0
B	8	HIS	-	expression tag	UNP S8ESX0
B	9	HIS	-	expression tag	UNP S8ESX0
B	10	HIS	-	expression tag	UNP S8ESX0
B	11	HIS	-	expression tag	UNP S8ESX0
B	12	HIS	-	expression tag	UNP S8ESX0
B	13	SER	-	expression tag	UNP S8ESX0
B	14	SER	-	expression tag	UNP S8ESX0
B	15	GLY	-	expression tag	UNP S8ESX0
B	16	HIS	-	expression tag	UNP S8ESX0
B	17	ILE	-	expression tag	UNP S8ESX0
B	18	GLU	-	expression tag	UNP S8ESX0
B	19	GLY	-	expression tag	UNP S8ESX0
B	20	ARG	-	expression tag	UNP S8ESX0
B	21	HIS	-	expression tag	UNP S8ESX0
B	22	MET	-	expression tag	UNP S8ESX0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

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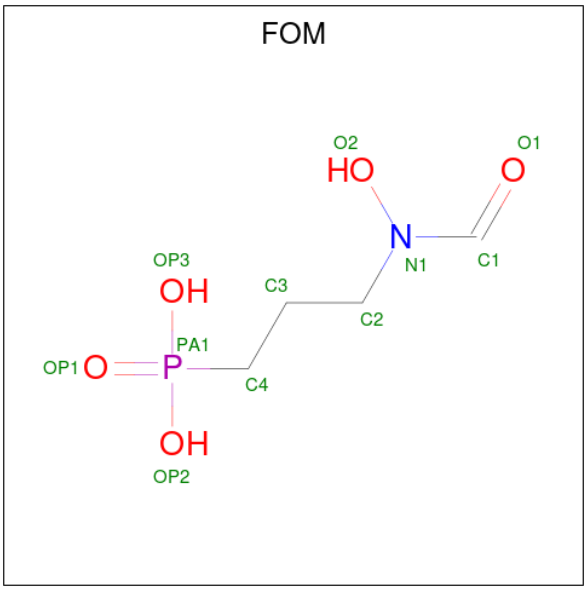
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

- Molecule 3 is 3-[FORMYL(HYDROXY)AMINO]PROPYLPHOSPHONIC ACID (three-letter code: FOM) (formula: $C_4H_{10}NO_5P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			19	4	8	1	5	1		
3	B	1	Total	C	H	N	O	P	0	0
			19	4	8	1	5	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is water.

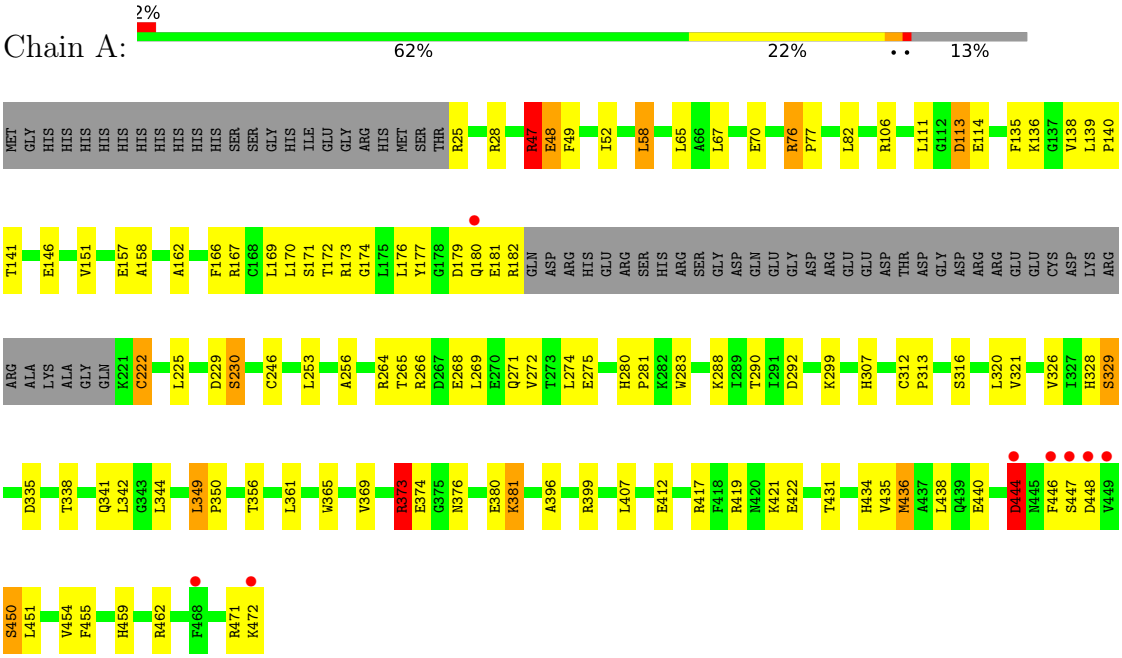
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total O 5 5	0	0
6	B	4	Total O 4 4	0	0

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.

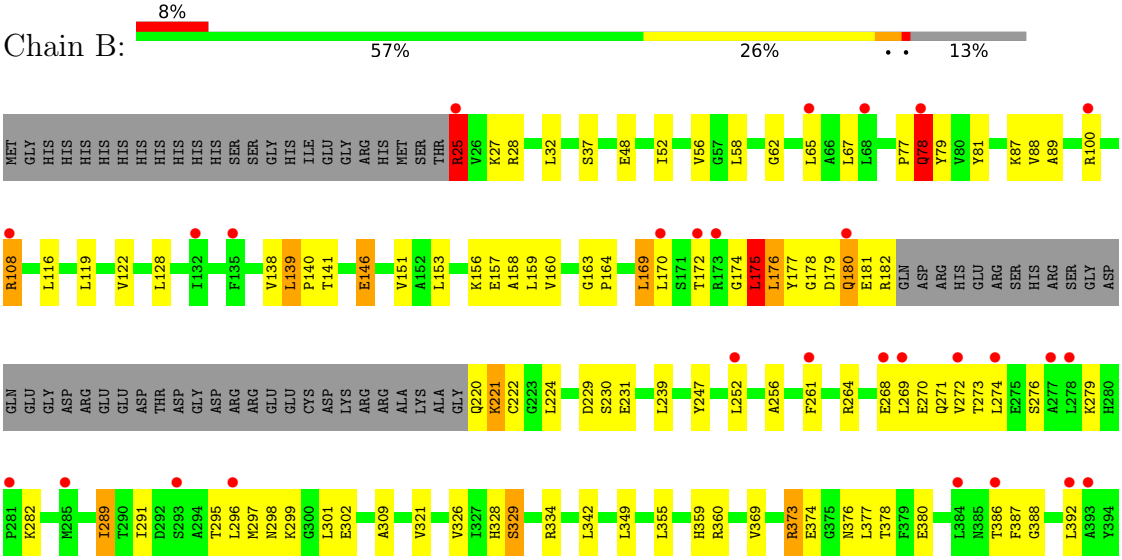
• Molecule 1: 1-deoxy-D-xylulose-5-phosphate reductoisomerase

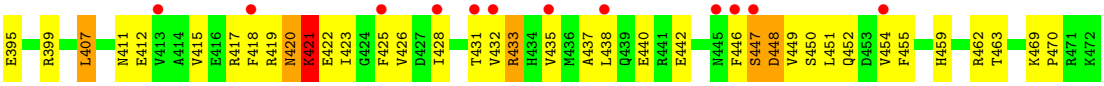
Chain A:



• Molecule 1: 1-deoxy-D-xylulose-5-phosphate reductoisomerase

Chain B:




E395
R399
L407
N411
E412
V413
A414
V415
E416
R417
F418
R419
N420
K421
E422
I423
G424
F425
V426
D427
I428
T431
V432
R433
H434
V435
M436
A437
L438
Q439
E440
R441
E442
N445
F446
S447
D448
V449
S450
L451
Q452
D453
V454
F455
H459
R462
T463
K469
P470
R471
K472

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	159.52Å 159.52Å 75.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.50 – 2.56 66.50 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.0 (66.50-2.56) 99.0 (66.50-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.194 , 0.225 0.194 , 0.226	Depositor DCC
R_{free} test set	2004 reflections (5.66%)	wwPDB-VP
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12821	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, FOM, MG, NAP

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	0.74	6/3195 (0.2%)	0.90	9/4333 (0.2%)
1	B	1.12	27/3215 (0.8%)	1.41	40/4359 (0.9%)
All	All	0.95	33/6410 (0.5%)	1.18	49/8692 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	GLN	CG-CD	17.10	1.90	1.51
1	B	169	LEU	CG-CD2	16.14	2.11	1.51
1	B	25	ARG	CG-CD	15.45	1.90	1.51
1	B	373	ARG	CZ-NH1	13.45	1.50	1.33
1	B	25	ARG	CB-CG	12.79	1.87	1.52
1	A	381	LYS	CE-NZ	12.15	1.79	1.49
1	B	421	LYS	CB-CG	11.77	1.84	1.52
1	B	373	ARG	CG-CD	11.21	1.79	1.51
1	A	381	LYS	CD-CE	-10.88	1.24	1.51
1	B	175	LEU	CG-CD2	10.27	1.89	1.51
1	B	108	ARG	CZ-NH2	9.33	1.45	1.33
1	B	78	GLN	CD-OE1	-9.18	1.03	1.24
1	B	373	ARG	CZ-NH2	9.17	1.45	1.33
1	B	469	LYS	CD-CE	8.35	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	GLN	CB-CG	8.21	1.74	1.52
1	B	108	ARG	CG-CD	-8.08	1.31	1.51
1	B	78	GLN	CD-NE2	7.37	1.51	1.32
1	B	289	ILE	CB-CG2	7.15	1.75	1.52
1	A	222	CYS	CB-SG	-6.89	1.70	1.82
1	B	25	ARG	NE-CZ	6.66	1.41	1.33
1	A	246	CYS	CB-SG	-6.54	1.71	1.82
1	A	114	GLU	CD-OE1	6.32	1.32	1.25
1	B	146	GLU	CD-OE2	6.32	1.32	1.25
1	B	108	ARG	CZ-NH1	6.25	1.41	1.33
1	B	421	LYS	CE-NZ	5.97	1.64	1.49
1	B	25	ARG	CD-NE	5.91	1.56	1.46
1	B	25	ARG	CZ-NH2	5.88	1.40	1.33
1	B	421	LYS	C-O	-5.87	1.12	1.23
1	B	469	LYS	CG-CD	5.79	1.72	1.52
1	B	395	GLU	CD-OE1	5.74	1.31	1.25
1	B	462	ARG	CG-CD	5.44	1.65	1.51
1	B	373	ARG	CB-CG	5.40	1.67	1.52
1	A	436	MET	CG-SD	-5.20	1.67	1.81

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	LEU	CB-CG-CD2	-24.50	69.35	111.00
1	B	108	ARG	NE-CZ-NH1	-22.48	109.06	120.30
1	B	373	ARG	NE-CZ-NH1	-22.09	109.25	120.30
1	B	169	LEU	CB-CG-CD1	18.14	141.84	111.00
1	B	108	ARG	NH1-CZ-NH2	17.99	139.19	119.40
1	B	108	ARG	NE-CZ-NH2	-17.29	111.66	120.30
1	B	169	LEU	CB-CG-CD2	-16.32	83.26	111.00
1	B	175	LEU	CB-CG-CD1	15.03	136.56	111.00
1	B	25	ARG	NE-CZ-NH1	14.90	127.75	120.30
1	B	25	ARG	CD-NE-CZ	13.88	143.03	123.60
1	B	462	ARG	NE-CZ-NH2	12.17	126.39	120.30
1	A	47	ARG	CG-CD-NE	11.73	136.44	111.80
1	B	78	GLN	CG-CD-OE1	-10.48	100.64	121.60
1	B	67	LEU	CB-CG-CD1	9.80	127.66	111.00
1	A	373	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	B	462	ARG	NE-CZ-NH1	-9.74	115.43	120.30
1	B	25	ARG	N-CA-C	-9.73	84.74	111.00
1	B	373	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	B	373	ARG	CD-NE-CZ	8.93	136.10	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	421	LYS	CA-CB-CG	8.82	132.81	113.40
1	B	25	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	67	LEU	CB-CG-CD2	-8.06	97.30	111.00
1	B	25	ARG	NH1-CZ-NH2	-7.76	110.86	119.40
1	B	108	ARG	CG-CD-NE	-7.67	95.70	111.80
1	B	25	ARG	CB-CG-CD	7.53	131.18	111.60
1	B	169	LEU	CA-CB-CG	7.48	132.50	115.30
1	B	462	ARG	CG-CD-NE	7.15	126.81	111.80
1	B	373	ARG	CB-CG-CD	7.10	130.07	111.60
1	A	444	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	B	421	LYS	CD-CE-NZ	-6.76	96.14	111.70
1	B	78	GLN	N-CA-CB	-6.66	98.62	110.60
1	B	433	ARG	CA-CB-CG	-6.64	98.78	113.40
1	B	433	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	436	MET	CA-CB-CG	-6.47	102.31	113.30
1	A	76	ARG	CG-CD-NE	6.42	125.28	111.80
1	A	381	LYS	CD-CE-NZ	-6.39	96.99	111.70
1	A	111	LEU	CB-CG-CD1	-6.20	100.45	111.00
1	B	395	GLU	CB-CG-CD	-5.94	98.17	114.20
1	B	176	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	B	373	ARG	NH1-CZ-NH2	5.73	125.70	119.40
1	B	252	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	289	ILE	CA-CB-CG1	5.38	121.22	111.00
1	B	25	ARG	CA-CB-CG	5.36	125.19	113.40
1	A	349	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	B	395	GLU	CA-CB-CG	5.24	124.94	113.40
1	B	289	ILE	CG1-CB-CG2	-5.07	100.24	111.40
1	B	469	LYS	CA-CB-CG	-5.07	102.24	113.40
1	B	469	LYS	CG-CD-CE	-5.05	96.74	111.90
1	A	58	LEU	CB-CG-CD1	-5.01	102.47	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	B	146	GLU	Sidechain
1	B	25	ARG	Sidechain
1	B	420	ASN	Peptide
1	B	447	SER	Peptide
1	B	78	GLN	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3133	3159	3159	81	1
1	B	3150	3180	3179	156	1
2	A	48	25	24	1	0
2	B	48	25	24	4	0
3	A	11	8	8	2	0
3	B	11	8	8	1	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	2	0
6	B	4	0	0	0	0
All	All	6416	6405	6402	235	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 18.

All (235) 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:373:ARG:CG	1:B:373:ARG:CD	1.80	1.59
1:B:78:GLN:CB	1:B:78:GLN:CG	1.74	1.57
1:B:289:ILE:CG2	1:B:289:ILE:CB	1.75	1.57
1:B:421:LYS:CG	1:B:421:LYS:CB	1.84	1.55
1:B:25:ARG:CG	1:B:25:ARG:CB	1.87	1.53
1:B:25:ARG:CG	1:B:25:ARG:CD	1.90	1.48
1:B:175:LEU:CG	1:B:175:LEU:CD2	1.89	1.48
1:A:381:LYS:CE	1:A:381:LYS:NZ	1.79	1.44
1:B:78:GLN:CG	1:B:78:GLN:CD	1.90	1.40
1:B:175:LEU:CD2	1:B:175:LEU:CB	1.97	1.40
1:B:169:LEU:CG	1:B:169:LEU:CD2	2.11	1.28
2:A:501:NAP:O4D	2:A:501:NAP:C1D	1.64	1.27
2:B:501:NAP:O4B	2:B:501:NAP:C1B	1.64	1.22
1:B:172:THR:OG1	1:B:181:GLU:OE1	1.56	1.16
1:B:175:LEU:CD2	1:B:175:LEU:HB3	1.72	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:HB3	1:B:175:LEU:HD22	1.40	0.98
1:B:56:VAL:HG12	1:B:78:GLN:NE2	1.78	0.96
1:A:381:LYS:NZ	1:A:381:LYS:CD	2.30	0.94
1:B:169:LEU:CD2	1:B:169:LEU:CB	2.46	0.93
1:B:175:LEU:CA	1:B:175:LEU:HD23	2.01	0.90
1:A:172:THR:HG22	1:A:174:GLY:H	1.36	0.89
1:A:356:THR:HG21	1:A:361:LEU:HD13	1.55	0.88
1:B:139:LEU:H	1:B:139:LEU:HD23	1.39	0.87
1:B:289:ILE:CG2	1:B:289:ILE:CG1	2.52	0.86
1:B:175:LEU:CD2	1:B:175:LEU:CA	2.55	0.84
1:B:169:LEU:CD2	1:B:169:LEU:CA	2.54	0.84
1:B:169:LEU:CD2	1:B:169:LEU:HA	2.06	0.84
1:B:175:LEU:HD23	1:B:175:LEU:C	1.99	0.82
1:B:289:ILE:HG21	1:B:289:ILE:HD13	1.62	0.81
1:B:78:GLN:CG	1:B:78:GLN:OE1	2.32	0.78
1:B:296:LEU:HD12	1:B:387:PHE:CG	2.19	0.77
1:B:291:ILE:O	1:B:295:THR:HG23	1.85	0.77
1:B:78:GLN:CG	1:B:78:GLN:CA	2.63	0.77
1:A:288:LYS:NZ	6:A:601:HOH:O	2.18	0.75
1:A:256:ALA:HB2	1:A:299:LYS:HG3	1.67	0.75
1:B:56:VAL:HG12	1:B:78:GLN:HE21	1.50	0.75
1:B:175:LEU:HG	1:B:247:TYR:OH	1.88	0.74
1:B:229:ASP:OD1	2:B:501:NAP:H6N	1.86	0.74
1:B:139:LEU:HG	1:B:140:PRO:HD3	1.67	0.74
1:B:56:VAL:CG1	1:B:78:GLN:HE21	2.01	0.72
1:B:296:LEU:HD12	1:B:387:PHE:CB	2.19	0.72
1:B:289:ILE:CG2	1:B:289:ILE:CA	2.67	0.72
1:B:256:ALA:HB2	1:B:299:LYS:HG3	1.72	0.71
1:B:56:VAL:CB	1:B:78:GLN:HE21	2.04	0.71
1:A:172:THR:HG21	4:A:503:CL:CL	2.28	0.70
1:B:373:ARG:CG	1:B:373:ARG:NE	2.54	0.69
1:B:433:ARG:HG2	1:B:433:ARG:HH11	1.55	0.69
1:B:175:LEU:CD2	1:B:175:LEU:CD1	2.70	0.69
1:A:106:ARG:NH2	6:A:602:HOH:O	2.27	0.68
1:B:169:LEU:HA	1:B:169:LEU:HD23	1.76	0.68
1:B:164:PRO:CB	1:B:449:VAL:HG21	2.24	0.67
1:B:25:ARG:HH12	1:B:52:ILE:HG12	1.59	0.67
1:A:179:ASP:OD1	1:A:180:GLN:NE2	2.28	0.67
1:B:153:LEU:HD21	1:B:159:LEU:HD23	1.77	0.66
1:B:282:LYS:HE3	1:B:282:LYS:HA	1.78	0.65
1:B:296:LEU:HD12	1:B:387:PHE:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LYS:HD3	1:B:222:CYS:H	1.61	0.65
1:B:264:ARG:HA	1:B:264:ARG:NE	2.11	0.65
1:B:56:VAL:HG12	1:B:78:GLN:HE22	1.61	0.65
1:B:100:ARG:HA	1:B:100:ARG:HE	1.62	0.64
1:B:56:VAL:CG1	1:B:78:GLN:NE2	2.56	0.64
1:B:272:VAL:HG11	1:B:425:PHE:HB2	1.79	0.64
1:B:169:LEU:CD2	1:B:169:LEU:CD1	2.76	0.63
1:B:169:LEU:CA	1:B:169:LEU:HD22	2.28	0.62
1:A:146:GLU:HG3	1:A:169:LEU:HD11	1.80	0.62
1:B:438:LEU:O	1:B:442:GLU:HB2	1.99	0.62
1:B:139:LEU:HG	1:B:140:PRO:CD	2.29	0.62
1:A:344:LEU:HG	1:A:369:VAL:HG22	1.81	0.62
1:B:172:THR:CG2	1:B:181:GLU:OE1	2.48	0.62
1:A:407:LEU:HD12	1:A:436:MET:HE1	1.82	0.61
1:B:32:LEU:HG	1:B:128:LEU:HD11	1.81	0.61
1:B:170:LEU:HD12	1:B:176:LEU:HD22	1.83	0.60
1:B:58:LEU:HD12	1:B:77:PRO:HG3	1.82	0.60
1:B:56:VAL:HB	1:B:78:GLN:HE21	1.66	0.60
1:B:27:LYS:HE3	1:B:355:LEU:O	2.02	0.59
1:B:274:LEU:HD13	1:B:419:ARG:HA	1.84	0.59
1:A:349:LEU:HB3	1:A:350:PRO:HD3	1.84	0.59
1:B:220:GLN:CD	1:B:221:LYS:H	2.05	0.59
1:B:175:LEU:HG	1:B:247:TYR:CZ	2.38	0.59
1:B:175:LEU:HD23	1:B:176:LEU:N	2.18	0.59
1:A:341:GLN:NE2	1:A:342:LEU:O	2.36	0.58
1:B:179:ASP:OD1	1:B:180:GLN:N	2.35	0.58
1:A:349:LEU:HB3	1:A:350:PRO:CD	2.32	0.58
1:A:58:LEU:HD12	1:A:77:PRO:HG3	1.85	0.58
1:B:141:THR:HG23	1:B:151:VAL:HG11	1.86	0.58
1:B:100:ARG:HA	1:B:100:ARG:NE	2.18	0.58
1:B:289:ILE:HG21	1:B:289:ILE:CD1	2.34	0.58
1:B:25:ARG:NH1	1:B:52:ILE:HG12	2.18	0.57
1:A:169:LEU:O	1:A:169:LEU:HD23	2.03	0.56
1:A:321:VAL:HB	1:A:380:GLU:HG2	1.87	0.56
1:A:356:THR:HG21	1:A:361:LEU:CD1	2.31	0.56
1:B:169:LEU:HA	1:B:169:LEU:HD22	1.85	0.56
1:B:420:ASN:O	1:B:422:GLU:HG3	2.05	0.56
1:B:289:ILE:CG2	1:B:289:ILE:CD1	2.83	0.56
1:B:411:ASN:O	1:B:415:VAL:HG23	2.07	0.55
1:B:282:LYS:HE3	1:B:282:LYS:CA	2.36	0.55
1:B:229:ASP:OD1	2:B:501:NAP:C6N	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:VAL:HG21	1:B:374:GLU:HG2	1.88	0.55
1:A:341:GLN:HE21	1:A:342:LEU:N	2.03	0.55
1:A:326:VAL:HG21	1:A:374:GLU:HG2	1.90	0.54
1:B:79:TYR:CE1	1:B:108:ARG:CZ	2.90	0.54
1:A:138:VAL:HG22	1:A:158:ALA:HA	1.89	0.54
1:B:437:ALA:O	1:B:440:GLU:HB2	2.08	0.54
1:B:164:PRO:CB	1:B:449:VAL:CG2	2.86	0.53
1:A:307:HIS:HD2	1:A:312:CYS:O	1.91	0.53
1:B:172:THR:HG22	1:B:174:GLY:H	1.73	0.53
1:B:65:LEU:HD11	1:B:87:LYS:HB3	1.91	0.53
1:B:417:ARG:HG2	1:B:422:GLU:OE2	2.09	0.53
1:B:433:ARG:HH11	1:B:433:ARG:CG	2.22	0.53
1:B:172:THR:CB	1:B:181:GLU:OE1	2.54	0.53
1:B:261:PHE:HZ	1:B:276:SER:HB2	1.74	0.53
1:B:274:LEU:HD12	1:B:418:PHE:CE1	2.44	0.53
1:B:279:LYS:HD3	1:B:279:LYS:O	2.09	0.53
1:B:433:ARG:HG2	1:B:433:ARG:NH1	2.23	0.53
1:B:156:LYS:HE3	1:B:302:GLU:OE1	2.09	0.52
1:B:421:LYS:CB	1:B:421:LYS:CD	2.82	0.52
1:A:49:PHE:HB3	1:A:52:ILE:HD12	1.92	0.52
1:B:256:ALA:HB2	1:B:299:LYS:CG	2.40	0.52
1:B:229:ASP:HA	2:B:501:NAP:H5N	1.92	0.52
1:B:175:LEU:HD11	1:B:239:LEU:HD13	1.92	0.52
1:B:386:THR:HG1	1:B:387:PHE:HD1	1.58	0.52
1:A:167:ARG:HD2	1:A:173:ARG:HA	1.92	0.52
1:B:433:ARG:CG	1:B:433:ARG:NH1	2.72	0.52
1:A:376:ASN:HD22	1:B:376:ASN:ND2	2.08	0.51
1:A:169:LEU:CD2	1:A:222:CYS:SG	2.98	0.51
1:B:431:THR:O	1:B:435:VAL:HG23	2.10	0.51
1:A:172:THR:HG22	1:A:174:GLY:N	2.16	0.51
1:B:160:VAL:HG21	1:B:301:LEU:HD22	1.93	0.51
1:A:328:HIS:O	1:A:329:SER:CB	2.59	0.51
1:B:169:LEU:HD13	1:B:222:CYS:SG	2.51	0.51
1:A:177:TYR:HA	1:A:225:LEU:O	2.10	0.51
1:B:326:VAL:HG13	1:B:369:VAL:HG21	1.91	0.51
1:B:297:MET:SD	1:B:407:LEU:HD21	2.51	0.50
1:A:135:PHE:HE2	1:A:455:PHE:CE1	2.29	0.50
1:A:447:SER:OG	1:A:448:ASP:N	2.44	0.50
1:A:269:LEU:HA	1:A:272:VAL:CG1	2.41	0.50
1:A:65:LEU:HD21	1:A:82:LEU:HD11	1.94	0.50
1:A:113:ASP:OD1	1:A:113:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ALA:HB2	1:A:299:LYS:CG	2.41	0.49
1:B:172:THR:HG23	1:B:181:GLU:OE1	2.12	0.49
1:B:178:GLY:O	1:B:224:LEU:HD22	2.12	0.49
1:A:407:LEU:HD12	1:A:436:MET:CE	2.42	0.49
1:A:412:GLU:CD	1:A:462:ARG:HH22	2.16	0.49
1:B:291:ILE:HG23	1:B:425:PHE:HE1	1.77	0.49
1:B:273:THR:OG1	1:B:276:SER:N	2.44	0.48
1:A:313:PRO:HD2	1:A:316:SER:OG	2.13	0.48
1:A:280:HIS:HB2	1:A:290:THR:HG23	1.95	0.48
1:A:283:TRP:CD1	3:A:502:FOM:H32	2.48	0.48
1:B:62:GLY:HA2	1:B:65:LEU:HD21	1.94	0.48
1:B:448:ASP:OD1	1:B:448:ASP:O	2.32	0.48
1:B:139:LEU:H	1:B:139:LEU:CD2	2.14	0.47
1:B:452:GLN:HA	1:B:455:PHE:HB2	1.96	0.47
1:A:265:THR:HG23	1:A:268:GLU:OE1	2.15	0.47
1:B:450:SER:O	1:B:454:VAL:HG23	2.15	0.47
1:A:230:SER:HB3	3:A:502:FOM:C1	2.46	0.46
1:A:328:HIS:O	1:A:329:SER:OG	2.27	0.46
1:A:451:LEU:HG	1:A:455:PHE:HE2	1.81	0.46
1:A:396:ALA:CB	1:A:407:LEU:HD13	2.46	0.46
1:B:172:THR:CG2	1:B:174:GLY:H	2.29	0.46
1:A:265:THR:O	1:A:269:LEU:HG	2.15	0.46
1:B:88:VAL:HG13	1:B:89:ALA:N	2.31	0.46
1:A:269:LEU:HA	1:A:272:VAL:HG13	1.99	0.45
1:A:376:ASN:HB3	1:B:378:THR:HG22	1.97	0.45
1:B:423:ILE:HG22	1:B:470:PRO:HG3	1.99	0.45
1:A:407:LEU:HD12	1:A:436:MET:SD	2.57	0.45
1:B:62:GLY:HA2	1:B:65:LEU:CD2	2.47	0.45
1:B:164:PRO:HB2	1:B:449:VAL:CG2	2.46	0.45
1:B:295:THR:OG1	1:B:297:MET:HB3	2.17	0.45
1:B:274:LEU:CD1	1:B:419:ARG:HA	2.46	0.45
1:A:434:HIS:O	1:A:438:LEU:HG	2.17	0.45
1:B:231:GLU:OE2	3:B:502:FOM:H22	2.17	0.45
1:A:67:LEU:HA	1:A:70:GLU:HG2	1.99	0.44
1:B:270:GLU:CD	1:B:426:VAL:HG21	2.37	0.44
1:A:399:ARG:HD2	1:A:440:GLU:OE1	2.18	0.44
1:B:399:ARG:CZ	1:B:440:GLU:OE1	2.66	0.44
1:B:177:TYR:CE2	1:B:309:ALA:HB1	2.52	0.44
1:A:274:LEU:HD13	1:A:419:ARG:HA	1.98	0.44
1:B:79:TYR:CE1	1:B:108:ARG:NH2	2.85	0.44
1:B:138:VAL:HG22	1:B:158:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LEU:O	1:B:442:GLU:CB	2.64	0.44
1:A:48:GLU:HG3	1:A:365:TRP:CZ3	2.53	0.44
1:A:157:GLU:OE1	1:A:157:GLU:N	2.41	0.43
1:A:321:VAL:HB	1:A:380:GLU:CG	2.47	0.43
1:A:450:SER:O	1:A:454:VAL:HG23	2.19	0.43
1:B:157:GLU:HG2	1:B:412:GLU:OE1	2.17	0.43
1:B:172:THR:HG22	1:B:174:GLY:N	2.33	0.43
1:A:444:ASP:OD1	1:A:446:PHE:CE2	2.72	0.43
1:B:328:HIS:O	1:B:329:SER:CB	2.66	0.43
1:A:170:LEU:HD13	1:A:176:LEU:HD22	2.00	0.43
1:A:396:ALA:HB2	1:A:407:LEU:HD13	1.99	0.43
1:A:253:LEU:HD22	1:A:320:LEU:HD11	2.00	0.43
1:B:388:GLY:O	1:B:392:LEU:HG	2.19	0.43
1:A:139:LEU:N	1:A:140:PRO:HD2	2.34	0.43
1:A:338:THR:HB	1:B:342:LEU:HB2	2.01	0.43
1:B:164:PRO:HB3	1:B:449:VAL:HG21	1.99	0.43
1:B:446:PHE:HB3	1:B:448:ASP:OD1	2.19	0.43
1:A:182:ARG:HB2	1:A:182:ARG:CZ	2.49	0.43
1:A:288:LYS:HE3	1:A:292:ASP:OD2	2.19	0.43
1:B:420:ASN:O	1:B:422:GLU:CG	2.67	0.42
1:B:451:LEU:HG	1:B:455:PHE:CE2	2.54	0.42
1:B:270:GLU:HB2	1:B:271:GLN:NE2	2.34	0.42
1:A:271:GLN:O	1:A:271:GLN:NE2	2.53	0.42
1:B:48:GLU:OE2	1:B:48:GLU:O	2.37	0.42
1:B:81:TYR:CD2	1:B:116:LEU:HD13	2.55	0.42
1:B:279:LYS:HD3	1:B:279:LYS:C	2.39	0.42
1:A:162:ALA:O	1:A:166:PHE:HD1	2.03	0.42
1:B:270:GLU:OE2	1:B:426:VAL:HG21	2.20	0.42
1:A:141:THR:HG23	1:A:151:VAL:HG11	2.01	0.41
1:A:381:LYS:NZ	1:A:381:LYS:HD3	2.28	0.41
1:B:156:LYS:HE2	1:B:298:ASN:ND2	2.34	0.41
1:B:376:ASN:O	1:B:377:LEU:HD23	2.19	0.41
1:A:275:GLU:H	1:A:275:GLU:CD	2.24	0.41
1:B:459:HIS:O	1:B:463:THR:HG23	2.20	0.41
1:A:451:LEU:HG	1:A:455:PHE:CE2	2.54	0.41
1:B:428:ILE:O	1:B:432:VAL:HG23	2.19	0.41
1:A:171:SER:O	1:A:171:SER:OG	2.39	0.41
1:B:321:VAL:HB	1:B:380:GLU:HG3	2.02	0.41
1:B:451:LEU:HG	1:B:455:PHE:HE2	1.86	0.41
1:A:265:THR:HG23	1:A:268:GLU:CD	2.41	0.41
1:A:280:HIS:ND1	1:A:281:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD11	1:B:87:LYS:CB	2.51	0.41
1:B:163:GLY:N	1:B:164:PRO:CD	2.83	0.41
1:B:221:LYS:CE	1:B:221:LYS:HA	2.51	0.41
1:A:341:GLN:NE2	1:A:342:LEU:C	2.74	0.41
1:A:417:ARG:HG2	1:A:422:GLU:OE2	2.20	0.41
1:B:269:LEU:O	1:B:272:VAL:HG12	2.21	0.41
1:A:381:LYS:NZ	1:A:381:LYS:HD2	2.28	0.40
1:A:431:THR:O	1:A:435:VAL:HG23	2.22	0.40
1:B:261:PHE:CZ	1:B:276:SER:HB2	2.55	0.40
1:B:359:HIS:CG	1:B:360:ARG:N	2.90	0.40
1:A:335:ASP:OD2	1:B:349:LEU:CD1	2.69	0.40
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.96	0.40
1:B:164:PRO:HB2	1:B:449:VAL:HG23	2.03	0.40
1:A:264:ARG:NH2	1:A:268:GLU:OE2	2.54	0.40
1:B:119:LEU:O	1:B:122:VAL:HG22	2.22	0.40

All (1) 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:A:373:ARG:HH22	1:B:447:SER:H[3_565]	1.12	0.48

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	406/472 (86%)	393 (97%)	11 (3%)	2 (0%)	29	39
1	B	408/472 (86%)	392 (96%)	13 (3%)	3 (1%)	22	29
All	All	814/944 (86%)	785 (96%)	24 (3%)	5 (1%)	25	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	GLN
1	A	329	SER
1	B	448	ASP
1	A	181	GLU
1	B	329	SER

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	326/379 (86%)	309 (95%)	17 (5%)	23	31
1	B	328/379 (86%)	316 (96%)	12 (4%)	34	45
All	All	654/758 (86%)	625 (96%)	29 (4%)	28	38

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	28	ARG
1	A	47	ARG
1	A	48	GLU
1	A	76	ARG
1	A	113	ASP
1	A	136	LYS
1	A	229	ASP
1	A	230	SER
1	A	266	ARG
1	A	373	ARG
1	A	421	LYS
1	A	444	ASP
1	A	450	SER
1	A	459	HIS
1	A	471	ARG
1	A	472	LYS
1	B	25	ARG
1	B	28	ARG

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Mol	Chain	Res	Type
1	B	37	SER
1	B	139	LEU
1	B	175	LEU
1	B	182	ARG
1	B	221	LYS
1	B	230	SER
1	B	268	GLU
1	B	334	ARG
1	B	407	LEU
1	B	421	LYS

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	271	GLN
1	A	307	HIS
1	A	341	GLN
1	A	385	ASN
1	B	78	GLN
1	B	240	GLN
1	B	271	GLN
1	B	376	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FOM	B	502	-	9,10,10	4.13	2 (22%)	11,13,13	1.69	4 (36%)
3	FOM	A	502	-	9,10,10	3.78	3 (33%)	11,13,13	2.04	6 (54%)
2	NAP	A	501	5	45,52,52	4.53	17 (37%)	56,80,80	1.95	13 (23%)
2	NAP	B	501	-	45,52,52	4.60	13 (28%)	56,80,80	1.96	10 (17%)

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	FOM	B	502	-	-	5/7/9/9	-
3	FOM	A	502	-	-	5/7/9/9	-
2	NAP	A	501	5	-	5/31/67/67	0/5/5/5
2	NAP	B	501	-	-	5/31/67/67	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAP	O4B-C1B	17.05	1.64	1.41
2	A	501	NAP	O4D-C1D	17.04	1.64	1.41
2	B	501	NAP	O4D-C1D	15.27	1.62	1.41
2	A	501	NAP	C2D-C1D	-14.64	1.31	1.53
2	B	501	NAP	C2D-C1D	-13.94	1.32	1.53
2	A	501	NAP	O4B-C1B	13.93	1.60	1.41
3	B	502	FOM	PA1-C4	9.15	1.88	1.78
3	A	502	FOM	PA1-C4	8.29	1.87	1.78
3	B	502	FOM	C1-N1	8.05	1.46	1.34
2	B	501	NAP	C7N-N7N	7.29	1.46	1.33
3	A	502	FOM	C1-N1	7.24	1.45	1.34
2	A	501	NAP	C7N-N7N	6.71	1.45	1.33
2	A	501	NAP	O4D-C4D	-6.00	1.31	1.45
2	B	501	NAP	O4D-C4D	-5.92	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAP	O4B-C4B	-5.84	1.32	1.45
2	A	501	NAP	O4B-C4B	-5.52	1.32	1.45
2	B	501	NAP	O2D-C2D	4.25	1.53	1.43
2	A	501	NAP	P2B-O2B	3.93	1.66	1.59
2	B	501	NAP	P2B-O2B	3.30	1.65	1.59
2	A	501	NAP	O2D-C2D	3.13	1.50	1.43
2	B	501	NAP	C6A-N6A	3.11	1.45	1.34
2	B	501	NAP	O7N-C7N	-3.06	1.18	1.24
2	B	501	NAP	O3D-C3D	-2.91	1.36	1.43
2	A	501	NAP	O3B-C3B	-2.86	1.36	1.43
2	A	501	NAP	C3N-C7N	2.69	1.54	1.50
2	A	501	NAP	O7N-C7N	-2.66	1.19	1.24
2	A	501	NAP	C2A-N3A	2.57	1.36	1.32
2	B	501	NAP	C5A-C4A	-2.52	1.34	1.40
2	A	501	NAP	C6A-N6A	2.51	1.43	1.34
2	A	501	NAP	C2N-N1N	2.35	1.37	1.35
2	A	501	NAP	O3D-C3D	-2.31	1.37	1.43
2	B	501	NAP	C2A-N3A	2.27	1.35	1.32
2	A	501	NAP	C5A-C4A	-2.15	1.35	1.40
3	A	502	FOM	PA1-OP3	-2.09	1.50	1.54
2	A	501	NAP	PA-O5B	2.02	1.67	1.59

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAP	C5A-C6A-N6A	7.32	131.48	120.35
2	A	501	NAP	C5A-C6A-N6A	6.70	130.53	120.35
2	B	501	NAP	C1B-N9A-C4A	-5.56	116.88	126.64
2	A	501	NAP	C1B-N9A-C4A	-5.04	117.79	126.64
2	B	501	NAP	N3A-C2A-N1A	-4.84	121.12	128.68
2	B	501	NAP	N6A-C6A-N1A	-4.61	109.00	118.57
2	A	501	NAP	N6A-C6A-N1A	-4.55	109.12	118.57
2	A	501	NAP	N3A-C2A-N1A	-4.27	122.00	128.68
2	A	501	NAP	C6N-N1N-C2N	-3.91	118.41	121.97
2	A	501	NAP	O7N-C7N-N7N	-3.75	117.26	122.58
3	A	502	FOM	C3-C2-N1	3.74	118.77	111.07
2	A	501	NAP	C3N-C7N-N7N	3.31	121.72	117.75
2	B	501	NAP	O4D-C4D-C3D	3.17	111.38	105.11
2	B	501	NAP	O3B-C3B-C4B	-2.85	102.82	111.05
2	B	501	NAP	O5B-C5B-C4B	-2.84	99.20	108.99
3	B	502	FOM	PA1-C4-C3	-2.77	111.51	114.98
3	B	502	FOM	OP2-PA1-OP1	-2.66	105.36	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	FOM	O2-N1-C2	2.51	119.84	113.67
3	B	502	FOM	O1-C1-N1	-2.46	118.72	125.80
3	A	502	FOM	O1-C1-N1	-2.46	118.73	125.80
2	A	501	NAP	C2D-C3D-C4D	2.36	107.23	102.64
2	A	501	NAP	C2N-N1N-C1D	2.33	124.32	119.14
2	A	501	NAP	O2D-C2D-C3D	-2.31	104.34	111.82
2	A	501	NAP	O2D-C2D-C1D	2.27	119.23	110.85
2	B	501	NAP	O4D-C4D-C5D	-2.25	101.98	109.37
2	A	501	NAP	PN-O3-PA	-2.23	125.19	132.83
3	A	502	FOM	C4-C3-C2	-2.22	105.77	111.29
2	B	501	NAP	C3N-C7N-N7N	2.20	120.39	117.75
2	B	501	NAP	O4D-C1D-C2D	2.18	110.11	106.93
2	A	501	NAP	O2X-P2B-O2B	2.15	115.62	105.99
3	B	502	FOM	O2-N1-C2	2.09	118.81	113.67
3	A	502	FOM	OP2-PA1-C4	2.07	111.82	106.95
3	A	502	FOM	OP3-PA1-OP1	-2.06	106.95	112.39

There are no chirality outliers.

All (20) torsion outliers are listed below:

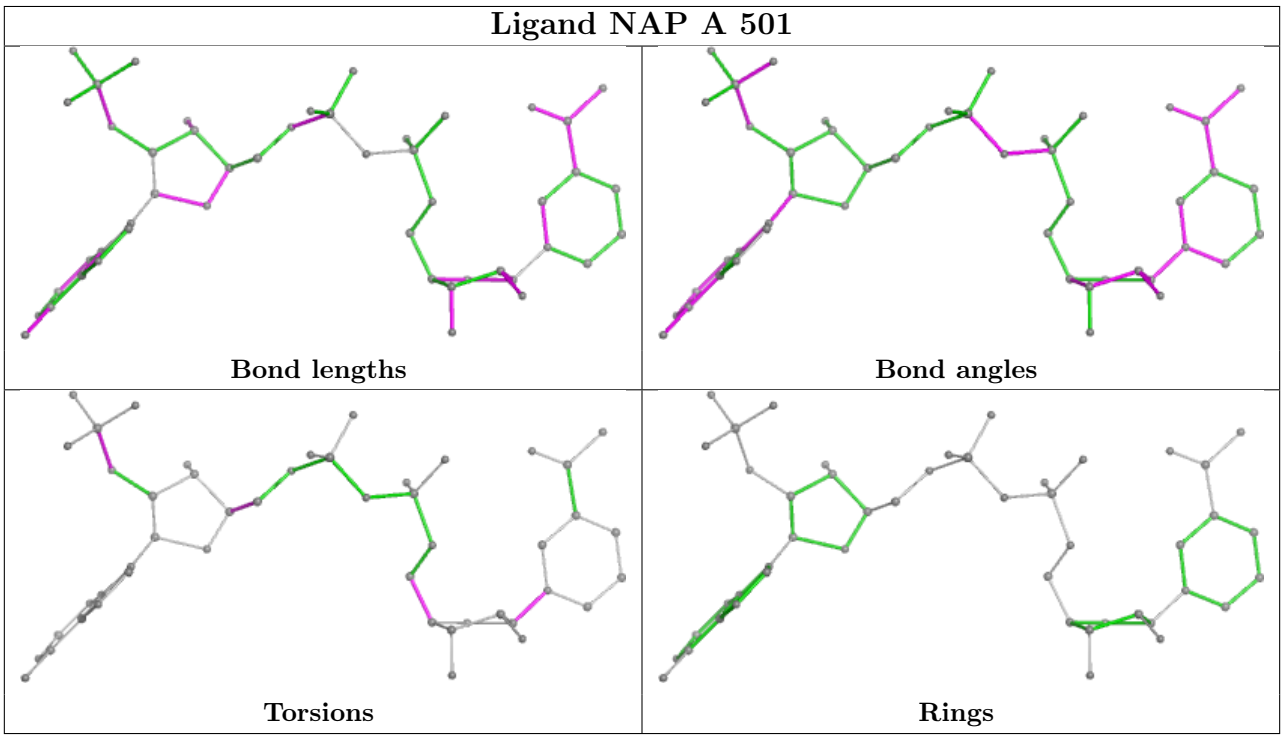
Mol	Chain	Res	Type	Atoms
2	A	501	NAP	O4D-C1D-N1N-C2N
2	B	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	O4D-C1D-N1N-C2N
3	A	502	FOM	C3-C2-N1-O2
3	A	502	FOM	N1-C2-C3-C4
3	A	502	FOM	C3-C4-PA1-OP1
3	A	502	FOM	C3-C4-PA1-OP2
3	A	502	FOM	C3-C4-PA1-OP3
3	B	502	FOM	C3-C2-N1-O2
3	B	502	FOM	N1-C2-C3-C4
3	B	502	FOM	C3-C4-PA1-OP1
3	B	502	FOM	C3-C4-PA1-OP2
3	B	502	FOM	C3-C4-PA1-OP3
2	B	501	NAP	C3B-C4B-C5B-O5B
2	A	501	NAP	O4B-C4B-C5B-O5B
2	A	501	NAP	C3B-C4B-C5B-O5B
2	B	501	NAP	C3B-C2B-O2B-P2B
2	A	501	NAP	C3D-C4D-C5D-O5D
2	A	501	NAP	C2B-O2B-P2B-O3X
2	B	501	NAP	C1B-C2B-O2B-P2B

There are no ring outliers.

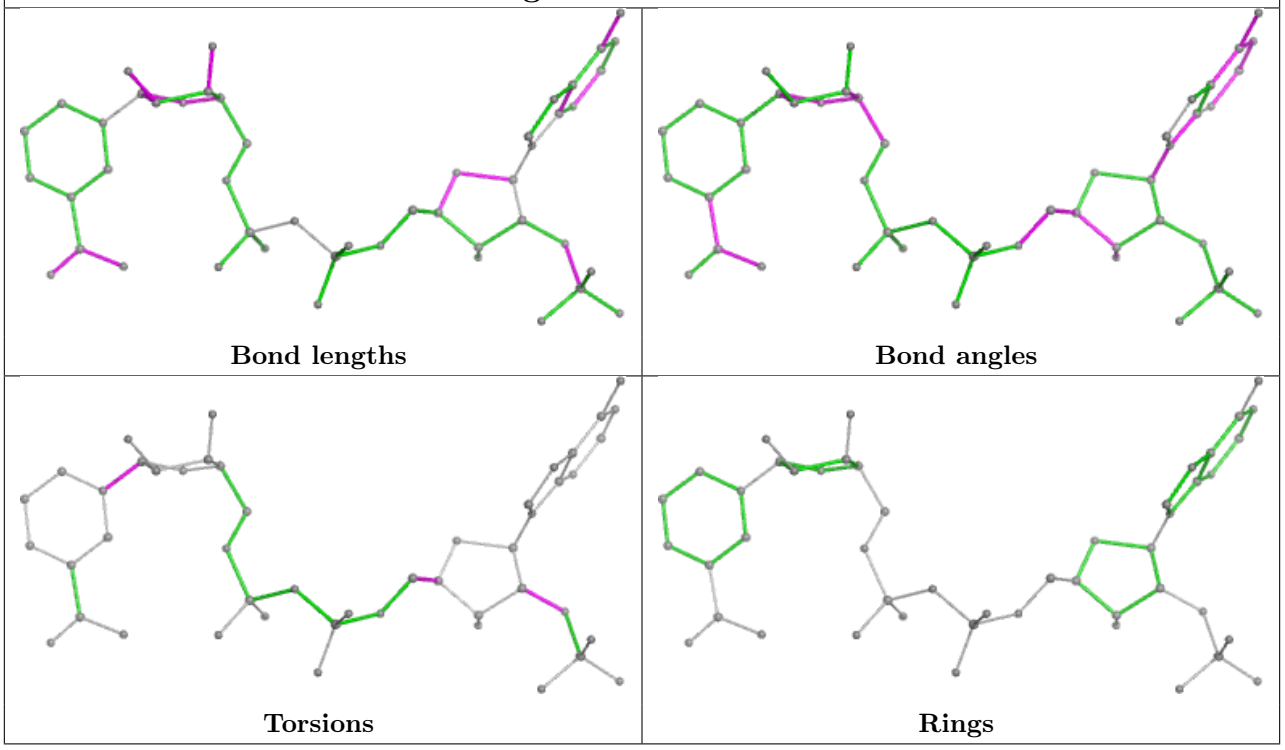
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	FOM	1	0
3	A	502	FOM	2	0
2	A	501	NAP	1	0
2	B	501	NAP	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand NAP B 501



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, 95^{th} 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	410/472 (86%)	0.41	8 (1%) 65 73	50, 68, 112, 175	0
1	B	411/472 (87%)	0.70	40 (9%) 7 11	50, 82, 130, 181	0
All	All	821/944 (86%)	0.56	48 (5%) 23 29	50, 73, 121, 181	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	PHE	9.2
1	B	425	PHE	8.7
1	B	277	ALA	5.1
1	B	447	SER	5.0
1	A	444	ASP	4.6
1	B	261	PHE	4.5
1	B	278	LEU	4.4
1	B	446	PHE	4.4
1	B	274	LEU	3.9
1	B	25	ARG	3.8
1	B	269	LEU	3.7
1	B	281	PRO	3.5
1	B	384	LEU	3.3
1	B	173	ARG	3.3
1	A	472	LYS	3.3
1	B	135	PHE	3.3
1	B	392	LEU	3.0
1	B	438	LEU	3.0
1	B	454	VAL	3.0
1	B	428	ILE	2.8
1	B	180	GLN	2.8
1	B	170	LEU	2.8
1	A	449	VAL	2.7
1	B	418	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	285	MET	2.6
1	B	432	VAL	2.5
1	B	431	THR	2.5
1	B	252	LEU	2.4
1	B	393	ALA	2.4
1	A	468	PHE	2.4
1	B	172	THR	2.4
1	B	435	VAL	2.4
1	A	447	SER	2.3
1	B	108	ARG	2.3
1	B	68	LEU	2.3
1	B	272	VAL	2.3
1	B	100	ARG	2.2
1	B	445	ASN	2.2
1	A	448	ASP	2.2
1	B	65	LEU	2.2
1	B	293	SER	2.2
1	B	78	GLN	2.1
1	B	268	GLU	2.1
1	A	180	GLN	2.1
1	B	132	ILE	2.1
1	B	386	THR	2.0
1	B	413	VAL	2.0
1	B	296	LEU	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)

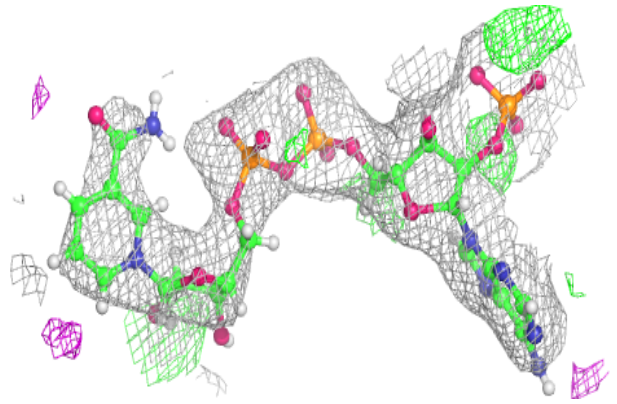
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

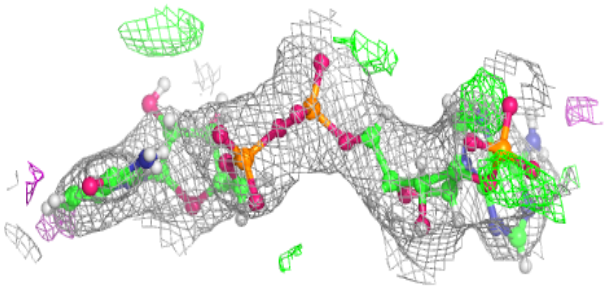
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	B	503	1/1	0.70	0.29	116,116,116,116	0
4	CL	A	503	1/1	0.75	0.16	113,113,113,113	0
5	MG	A	505	1/1	0.83	0.38	91,91,91,91	0
5	MG	B	504	1/1	0.84	0.39	69,69,69,69	0
2	NAP	B	501	48/48	0.87	0.22	71,105,138,146	0
3	FOM	B	502	11/11	0.90	0.21	92,109,130,130	0
5	MG	A	504	1/1	0.91	0.16	54,54,54,54	0
2	NAP	A	501	48/48	0.95	0.18	55,81,106,111	0
3	FOM	A	502	11/11	0.96	0.19	80,96,117,117	0
5	MG	A	506	1/1	0.97	0.21	77,77,77,77	0

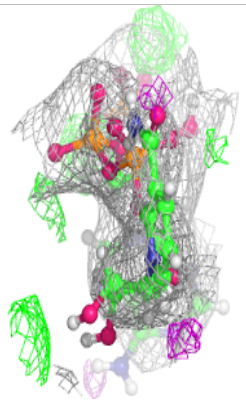
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP 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)

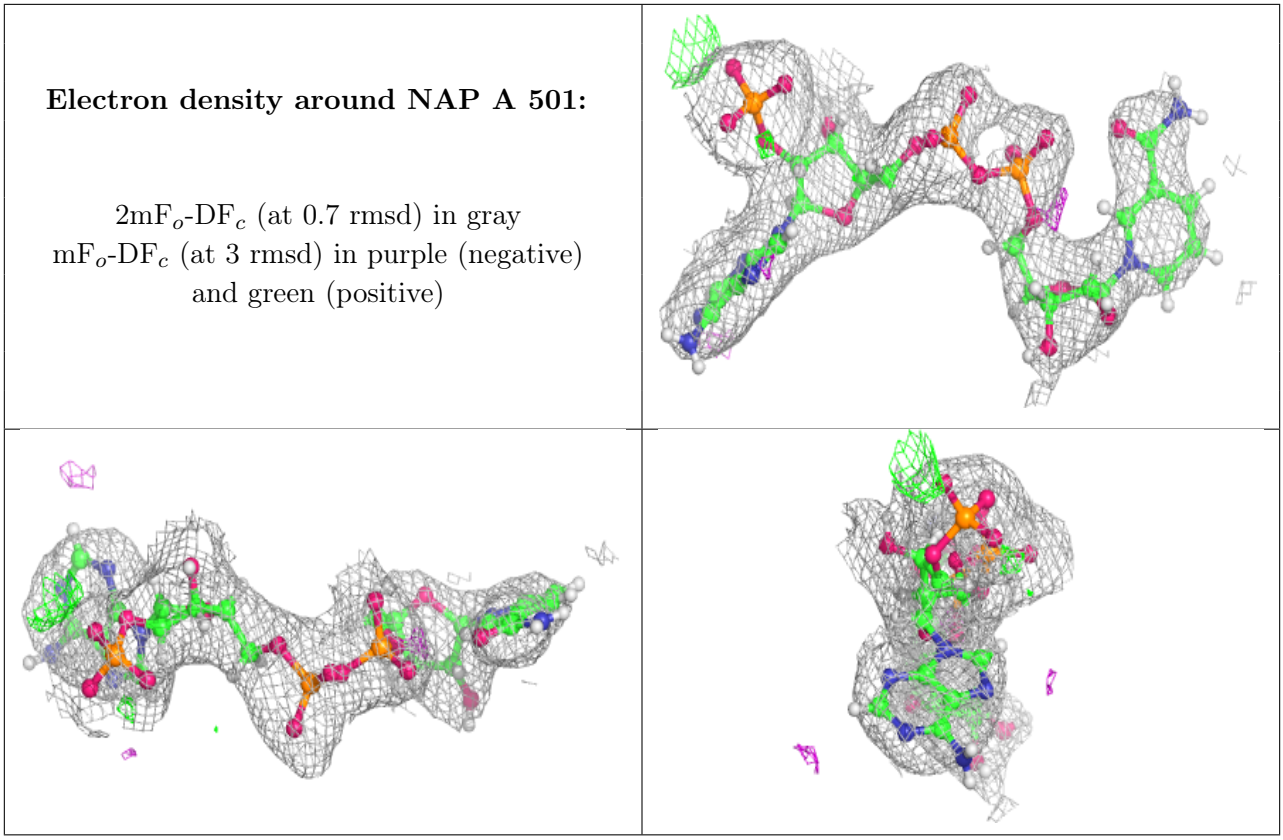






Electron density around NAP A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.