



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:49 pm GMT

PDB ID : 3CD2
Title : LIGAND INDUCED CONFORMATIONAL CHANGES IN THE CRYSTAL STRUCTURES OF PNEUMOCYSTIS CARINII DIHYDROFOLATE REDUCTASE COMPLEXES WITH FOLATE AND NADP+
Authors : Cody, V.; Galitsky, N.; Rak, D.; Luft, J.; Pangborn, W.; Queener, S.
Deposited on : 1999-03-16
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

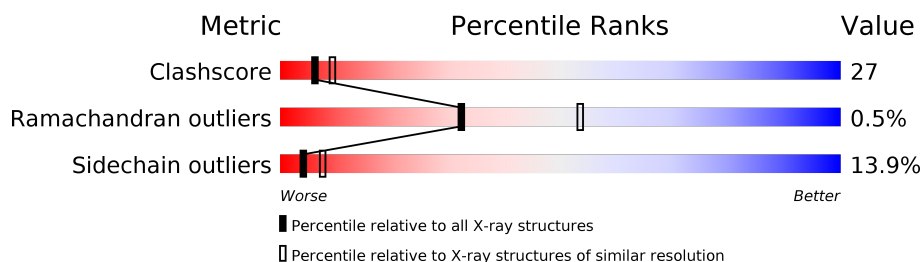
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	206	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1815 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 DIHYDROFOLATE REDUCTASE.

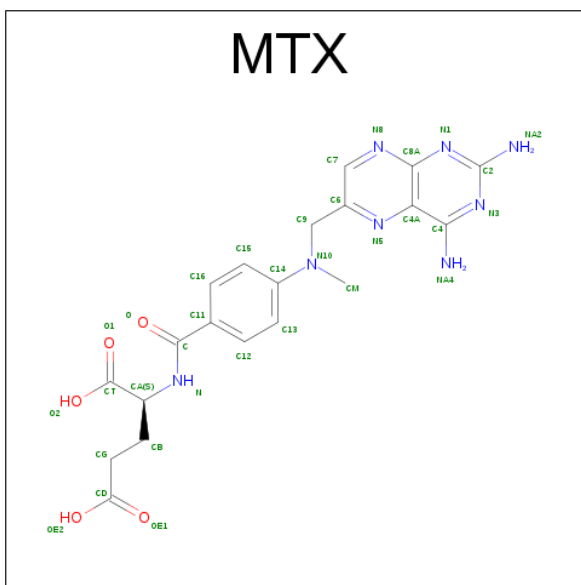
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1686	1086	288	305	7	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C₂₀H₂₂N₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 4 is water.

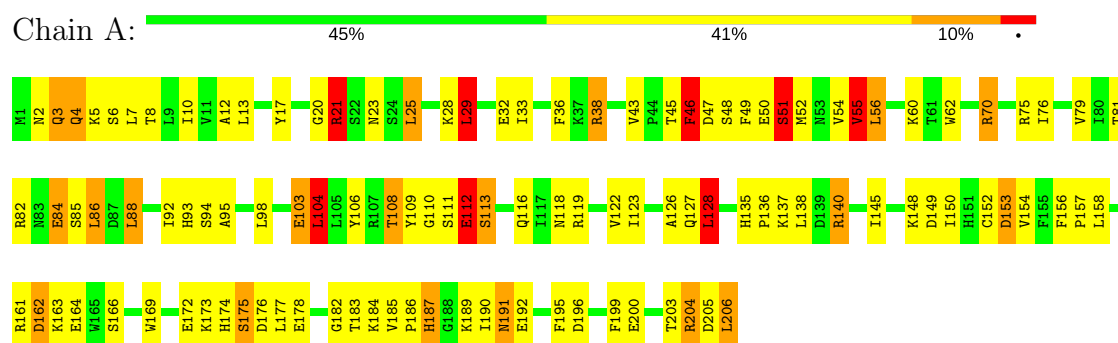
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	48	Total O 48 48	0	0

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.42 Å 43.56 Å 61.66 Å 90.00° 94.89° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.3 (8.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1815	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MTX, 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	4.47	1/1728 (0.1%)	2.35	64/2330 (2.7%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	PHE	C-O	182.30	4.69	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	O-C-N	-41.38	56.49	122.70
1	A	119	ARG	NE-CZ-NH1	26.61	133.61	120.30
1	A	204	ARG	CD-NE-CZ	25.98	159.96	123.60
1	A	38	ARG	NE-CZ-NH1	18.47	129.54	120.30
1	A	119	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	A	46	PHE	CA-C-O	13.58	148.61	120.10
1	A	140	ARG	NE-CZ-NH2	13.39	126.99	120.30
1	A	38	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	55	VAL	CB-CA-C	10.75	131.83	111.40
1	A	75	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	162	ASP	CB-CG-OD1	9.52	126.87	118.30
1	A	21	ARG	CD-NE-CZ	8.99	136.19	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	GLU	CA-CB-CG	8.76	132.68	113.40
1	A	140	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	A	50	GLU	OE1-CD-OE2	-8.29	113.35	123.30
1	A	56	LEU	CA-CB-CG	8.23	134.24	115.30
1	A	103	GLU	CA-CB-CG	8.07	131.15	113.40
1	A	21	ARG	CG-CD-NE	7.96	128.51	111.80
1	A	205	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	50	GLU	CG-CD-OE1	7.62	133.54	118.30
1	A	205	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	106	TYR	CB-CG-CD1	7.50	125.50	121.00
1	A	106	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	21	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	12	ALA	N-CA-CB	7.09	120.03	110.10
1	A	140	ARG	CD-NE-CZ	-7.01	113.78	123.60
1	A	192	GLU	CG-CD-OE2	-6.86	104.58	118.30
1	A	8	THR	N-CA-CB	6.85	123.32	110.30
1	A	38	ARG	CD-NE-CZ	6.80	133.12	123.60
1	A	161	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	206	LEU	CA-CB-CG	6.27	129.72	115.30
1	A	158	LEU	CB-CA-C	6.18	121.94	110.20
1	A	204	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	75	ARG	CD-NE-CZ	5.99	131.99	123.60
1	A	119	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
1	A	192	GLU	CG-CD-OE1	5.83	129.96	118.30
1	A	112	GLU	CA-CB-CG	5.83	126.22	113.40
1	A	108	THR	CA-CB-CG2	5.73	120.42	112.40
1	A	157	PRO	N-CA-C	5.73	127.00	112.10
1	A	55	VAL	N-CA-CB	-5.72	98.92	111.50
1	A	153	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	106	TYR	CB-CA-C	5.68	121.76	110.40
1	A	13	LEU	N-CA-CB	-5.67	99.06	110.40
1	A	70	ARG	CA-CB-CG	5.63	125.79	113.40
1	A	158	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	95	ALA	CB-CA-C	5.56	118.44	110.10
1	A	29	LEU	N-CA-CB	-5.52	99.36	110.40
1	A	55	VAL	CA-CB-CG1	5.51	119.17	110.90
1	A	112	GLU	OE1-CD-OE2	5.50	129.90	123.30
1	A	75	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	51	SER	N-CA-C	5.43	125.67	111.00
1	A	112	GLU	CG-CD-OE1	-5.30	107.71	118.30
1	A	79	VAL	CG1-CB-CG2	5.28	119.35	110.90
1	A	103	GLU	CB-CG-CD	5.26	128.40	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	LEU	N-CA-CB	-5.15	100.10	110.40
1	A	36	PHE	CB-CA-C	5.14	120.69	110.40
1	A	104	LEU	CB-CA-C	5.13	119.96	110.20
1	A	199	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	A	10	ILE	CB-CA-C	5.12	121.83	111.60
1	A	187	HIS	CB-CA-C	-5.12	100.16	110.40
1	A	175	SER	CB-CA-C	5.10	119.79	110.10
1	A	75	ARG	CA-CB-CG	5.10	124.62	113.40
1	A	200	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	A	156	PHE	CB-CA-C	5.01	120.41	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	PHE	Mainchain

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	1686	0	1693	94	1
2	A	48	0	25	4	0
3	A	33	0	20	5	0
4	A	48	0	0	5	0
All	All	1815	0	1738	95	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 27.

All (95) 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:A:148:LYS:HB3	1:A:150:ILE:HD11	1.30	1.07
1:A:7:LEU:HB3	1:A:138:LEU:HD23	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:N	1:A:150:ILE:HD12	1.92	0.84
1:A:122:VAL:HG13	1:A:128:LEU:HD13	1.61	0.83
1:A:46:PHE:O	1:A:47:ASP:CG	2.20	0.79
1:A:150:ILE:HD12	1:A:150:ILE:H	1.47	0.79
1:A:189:LYS:HB2	4:A:245:HOH:O	1.83	0.77
1:A:86:LEU:O	1:A:86:LEU:HD22	1.86	0.76
1:A:81:THR:HG23	1:A:84:GLU:HB2	1.68	0.75
1:A:82:ARG:HG3	2:A:207:NAP:H2A	1.67	0.74
1:A:28:LYS:CG	1:A:28:LYS:O	2.34	0.73
1:A:46:PHE:O	1:A:47:ASP:OD1	2.05	0.73
1:A:46:PHE:O	1:A:47:ASP:CB	2.37	0.72
1:A:175:SER:HB3	4:A:242:HOH:O	1.90	0.72
1:A:122:VAL:HG13	1:A:128:LEU:CD1	2.19	0.72
1:A:33:ILE:CG2	3:A:307:MTX:HB2	2.21	0.71
1:A:148:LYS:CB	1:A:150:ILE:HD11	2.16	0.70
1:A:135:HIS:HD2	1:A:137:LYS:H	1.40	0.70
1:A:104:LEU:HD12	1:A:104:LEU:C	2.12	0.69
1:A:38:ARG:NH2	1:A:185:VAL:HG22	2.07	0.69
1:A:186:PRO:HB2	1:A:190:ILE:HD11	1.75	0.69
1:A:122:VAL:CG1	1:A:128:LEU:HD13	2.25	0.67
1:A:45:THR:HA	1:A:48:SER:OG	1.96	0.66
1:A:81:THR:CG2	1:A:84:GLU:HB2	2.27	0.64
1:A:33:ILE:HG23	3:A:307:MTX:HB2	1.80	0.64
1:A:86:LEU:H	1:A:86:LEU:CD1	2.11	0.63
1:A:46:PHE:O	1:A:47:ASP:HB3	1.98	0.63
1:A:86:LEU:HD12	1:A:86:LEU:H	1.64	0.62
1:A:17:TYR:OH	1:A:162:ASP:OD1	2.14	0.61
1:A:82:ARG:CG	2:A:207:NAP:H2A	2.31	0.61
1:A:173:LYS:HG2	4:A:238:HOH:O	2.00	0.61
1:A:84:GLU:HG3	1:A:94:SER:OG	2.01	0.60
1:A:5:LYS:HE3	1:A:118:ASN:O	2.01	0.60
1:A:55:VAL:HG22	1:A:123:ILE:HG21	1.82	0.60
1:A:3:GLN:HG2	1:A:137:LYS:HG3	1.83	0.60
1:A:93:HIS:NE2	1:A:109:TYR:OH	2.33	0.59
1:A:191:ASN:HA	1:A:195:PHE:O	2.03	0.59
1:A:7:LEU:CB	1:A:138:LEU:HD23	2.24	0.58
1:A:110:GLY:O	1:A:113:SER:N	2.37	0.57
1:A:20:GLY:HA3	2:A:207:NAP:O3D	2.04	0.56
1:A:187:HIS:CE1	4:A:243:HOH:O	2.59	0.55
1:A:28:LYS:HG3	1:A:28:LYS:O	2.05	0.55
1:A:173:LYS:O	1:A:176:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:O	1:A:183:THR:OG1	2.26	0.54
1:A:3:GLN:HB3	1:A:137:LYS:HG3	1.90	0.54
1:A:86:LEU:N	1:A:86:LEU:CD1	2.71	0.54
1:A:43:VAL:HG22	1:A:118:ASN:OD1	2.08	0.53
1:A:54:VAL:HG22	1:A:76:ILE:HB	1.89	0.53
1:A:163:LYS:O	1:A:166:SER:OG	2.12	0.53
1:A:23:ASN:OD1	1:A:60:LYS:HE2	2.10	0.52
1:A:150:ILE:CD1	1:A:150:ILE:N	2.64	0.52
1:A:126:ALA:HB2	1:A:154:VAL:CG1	2.39	0.52
1:A:28:LYS:HG2	1:A:28:LYS:O	2.10	0.51
1:A:62:TRP:O	1:A:70:ARG:HD2	2.10	0.51
1:A:148:LYS:C	1:A:150:ILE:HD12	2.30	0.51
1:A:81:THR:OG1	2:A:207:NAP:O2X	2.19	0.51
1:A:21:ARG:HB2	1:A:152:CYS:HA	1.93	0.50
1:A:29:LEU:HB3	1:A:32:GLU:HB2	1.93	0.50
1:A:56:LEU:HD13	1:A:98:LEU:HD12	1.93	0.49
1:A:4:GLN:HA	1:A:4:GLN:HE21	1.77	0.49
1:A:150:ILE:CD1	1:A:150:ILE:H	2.23	0.49
1:A:104:LEU:CD1	1:A:104:LEU:C	2.80	0.48
1:A:110:GLY:O	1:A:112:GLU:N	2.46	0.48
1:A:25:LEU:HD21	3:A:307:MTX:C7	2.43	0.48
1:A:38:ARG:NH2	1:A:184:LYS:O	2.42	0.48
1:A:81:THR:HG23	1:A:84:GLU:CB	2.41	0.47
1:A:140:ARG:HG3	1:A:203:THR:HG22	1.97	0.47
1:A:169:TRP:CZ2	1:A:204:ARG:HD2	2.49	0.47
1:A:174:HIS:CE1	1:A:178:GLU:OE2	2.67	0.46
3:A:307:MTX:H15	3:A:307:MTX:HM1	1.69	0.46
1:A:153:ASP:HB2	4:A:248:HOH:O	2.15	0.46
1:A:47:ASP:C	1:A:49:PHE:H	2.18	0.46
1:A:86:LEU:O	1:A:86:LEU:HD13	2.16	0.45
1:A:148:LYS:C	1:A:150:ILE:CD1	2.85	0.45
1:A:62:TRP:CH2	1:A:70:ARG:HG2	2.52	0.45
1:A:174:HIS:HE1	1:A:178:GLU:OE2	2.01	0.44
1:A:135:HIS:CG	1:A:136:PRO:HD2	2.53	0.44
1:A:88:LEU:HD22	1:A:88:LEU:HA	1.77	0.43
1:A:113:SER:HB3	1:A:116:GLN:NE2	2.34	0.43
1:A:172:GLU:CA	1:A:172:GLU:OE1	2.66	0.42
1:A:174:HIS:O	1:A:177:LEU:HB3	2.20	0.42
1:A:110:GLY:O	1:A:113:SER:HB2	2.19	0.42
1:A:7:LEU:O	1:A:138:LEU:HD22	2.19	0.42
1:A:45:THR:O	1:A:48:SER:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD12	1:A:86:LEU:N	2.30	0.42
1:A:21:ARG:HA	1:A:153:ASP:OD1	2.20	0.42
1:A:25:LEU:HD21	3:A:307:MTX:H7	2.03	0.41
1:A:43:VAL:HG11	1:A:51:SER:HB2	2.02	0.41
1:A:4:GLN:HA	1:A:4:GLN:NE2	2.36	0.41
1:A:4:GLN:NE2	1:A:4:GLN:CA	2.84	0.41
1:A:62:TRP:CH2	1:A:92:ILE:HD13	2.56	0.41
1:A:110:GLY:C	1:A:112:GLU:N	2.74	0.40
1:A:182:GLY:C	1:A:183:THR:OG1	2.60	0.40
1:A:62:TRP:CZ2	1:A:70:ARG:HG2	2.57	0.40
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.20	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:3:GLN:NE2	1:A:164:GLU:O[2_556]	2.19	0.01

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	204/206 (99%)	188 (92%)	15 (7%)	1 (0%)	32 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	SER

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	187/187 (100%)	161 (86%)	26 (14%)	4 7

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	GLN
1	A	4	GLN
1	A	6	SER
1	A	21	ARG
1	A	25	LEU
1	A	29	LEU
1	A	51	SER
1	A	52	MET
1	A	55	VAL
1	A	84	GLU
1	A	85	SER
1	A	86	LEU
1	A	88	LEU
1	A	103	GLU
1	A	104	LEU
1	A	108	THR
1	A	112	GLU
1	A	113	SER
1	A	127	GLN
1	A	128	LEU
1	A	145	ILE
1	A	149	ASP
1	A	191	ASN
1	A	196	ASP
1	A	206	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	100	HIS
1	A	116	GLN
1	A	135	HIS
1	A	174	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	NAP	A	207	-	44,52,52	3.08	19 (43%)	51,80,80	2.37	19 (37%)
3	MTX	A	307	-	28,35,35	1.18	3 (10%)	36,49,49	1.47	6 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	207	-	-	0/27/67/67	0/5/5/5
3	MTX	A	307	-	-	0/19/25/25	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	NAP	O4B-C4B	-8.18	1.26	1.45
2	A	207	NAP	C5A-C4A	-3.97	1.31	1.40
3	A	307	MTX	C8A-N8	-3.04	1.32	1.37
2	A	207	NAP	O7N-C7N	-2.81	1.18	1.24
3	A	307	MTX	CB-CA	-2.63	1.49	1.53
2	A	207	NAP	C6N-C5N	-2.62	1.32	1.38
2	A	207	NAP	C2N-C3N	-2.58	1.35	1.39
2	A	207	NAP	O2D-C2D	-2.55	1.37	1.43
3	A	307	MTX	C2-NA2	-2.47	1.28	1.34
2	A	207	NAP	C6A-N1A	-2.06	1.28	1.37
2	A	207	NAP	P2B-O3X	-2.03	1.46	1.54
2	A	207	NAP	O4B-C1B	2.01	1.44	1.41
2	A	207	NAP	C6N-N1N	2.04	1.40	1.35
2	A	207	NAP	C2D-C3D	2.38	1.59	1.53
2	A	207	NAP	C6A-C5A	2.65	1.56	1.42
2	A	207	NAP	PA-O5B	2.75	1.70	1.59
2	A	207	NAP	O3B-C3B	3.19	1.50	1.43
2	A	207	NAP	C3B-C4B	3.87	1.63	1.53
2	A	207	NAP	O4D-C1D	5.55	1.48	1.41
2	A	207	NAP	C5N-C4N	6.03	1.50	1.38
2	A	207	NAP	P2B-O2B	7.55	1.72	1.59
2	A	207	NAP	C4N-C3N	9.04	1.54	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	C5N-C4N-C3N	-7.23	111.84	120.35
2	A	207	NAP	C4D-O4D-C1D	-4.62	104.85	109.77
2	A	207	NAP	O3B-C3B-C4B	-4.52	97.88	111.09
2	A	207	NAP	O5D-C5D-C4D	-3.41	96.92	109.00
3	A	307	MTX	N1-C2-N3	-3.35	122.57	127.46
2	A	207	NAP	C2D-C3D-C4D	-2.71	97.35	102.62
2	A	207	NAP	C5A-C6A-N6A	-2.55	115.27	120.47
2	A	207	NAP	O5B-C5B-C4B	-2.35	100.67	109.00
2	A	207	NAP	C5B-C4B-C3B	-2.35	106.35	115.29
2	A	207	NAP	C3B-C2B-C1B	-2.19	98.47	102.75
2	A	207	NAP	C2B-C3B-C4B	-2.16	97.05	101.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	NAP	O2B-C2B-C1B	-2.09	102.28	110.06
3	A	307	MTX	N8-C8A-N1	2.19	118.87	116.04
3	A	307	MTX	CM-N10-C9	2.28	120.36	114.18
3	A	307	MTX	CG-CB-CA	2.37	117.92	113.19
2	A	207	NAP	C6N-C5N-C4N	2.39	123.05	119.44
3	A	307	MTX	CB-CA-N	2.53	114.06	110.22
2	A	207	NAP	O2A-PA-O1A	2.74	126.44	112.28
2	A	207	NAP	C4A-C5A-N7A	2.84	112.15	109.41
2	A	207	NAP	O3X-P2B-O2X	3.36	121.16	107.61
2	A	207	NAP	C2N-C3N-C4N	3.78	122.57	118.26
2	A	207	NAP	C4B-O4B-C1B	3.97	113.99	109.77
2	A	207	NAP	N6A-C6A-N1A	4.19	127.07	118.77
3	A	307	MTX	C2-N1-C8A	4.80	120.76	115.16
2	A	207	NAP	N3A-C2A-N1A	4.83	133.06	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	207	NAP	4	0
3	A	307	MTX	5	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.