



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2017 – 01:49 AM EDT

PDB ID : 5MSV
Title : Structure of the phosphopantetheine modified PCP-R didomain of carboxylic acid reductase (CAR) in complex with NADP
Authors : Gahloth, D.; Leys, D.
Deposited on : unknown
Resolution : 2.34 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) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

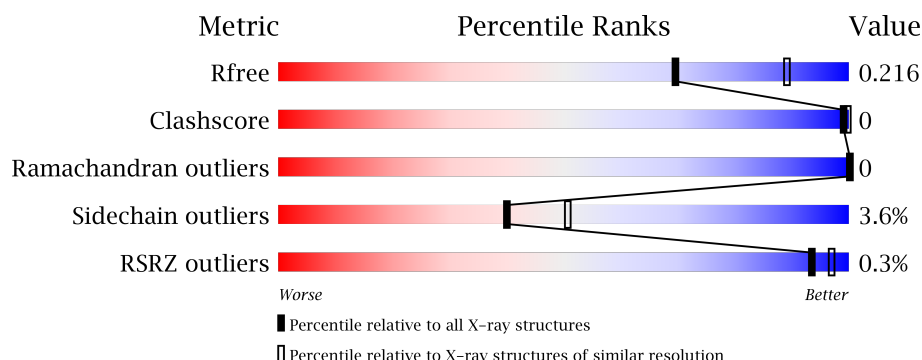
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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.

Mol	Chain	Length	Quality of chain
1	A	1188	
1	B	1188	
1	C	1188	
1	D	1188	

2 Entry composition [i](#)

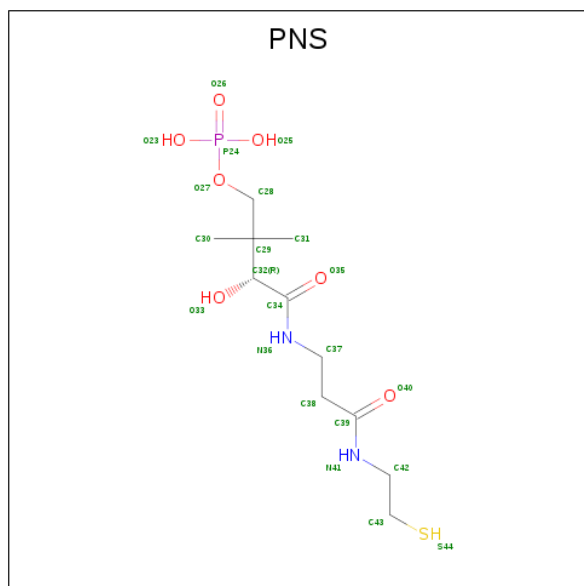
There are 4 unique types of molecules in this entry. The entry contains 16781 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thioester reductase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3932	2498	684	749	1			
1	B	514	Total	C	N	O	S	0	0	0
			3938	2500	687	750	1			
1	C	514	Total	C	N	O	S	0	0	0
			3938	2501	687	749	1			
1	D	515	Total	C	N	O	S	0	0	0
			3939	2500	688	750	1			

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS).



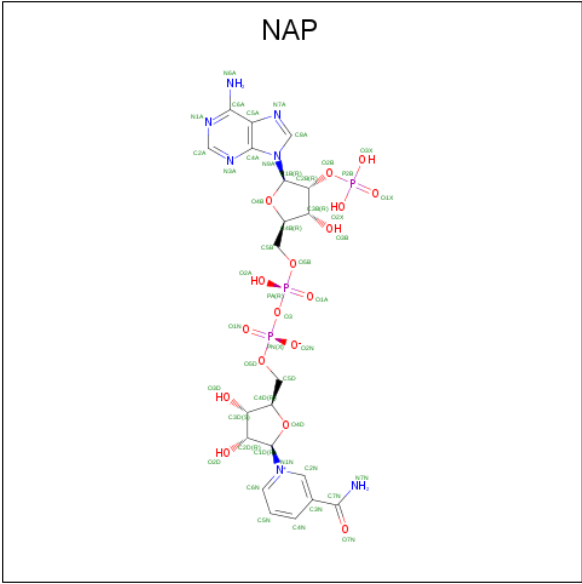
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	
2	B	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P		0	0
			40	15	6	16	3			
3	B	1	Total	C	N	O	P		0	0
			40	15	6	16	3			
3	C	1	Total	C	N	O	P		0	0
			40	15	6	16	3			
3	D	1	Total	C	N	O	P		0	0
			40	15	6	16	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	B	195	Total	O	0	0
			195	195		
4	C	164	Total	O	0	0
			164	164		

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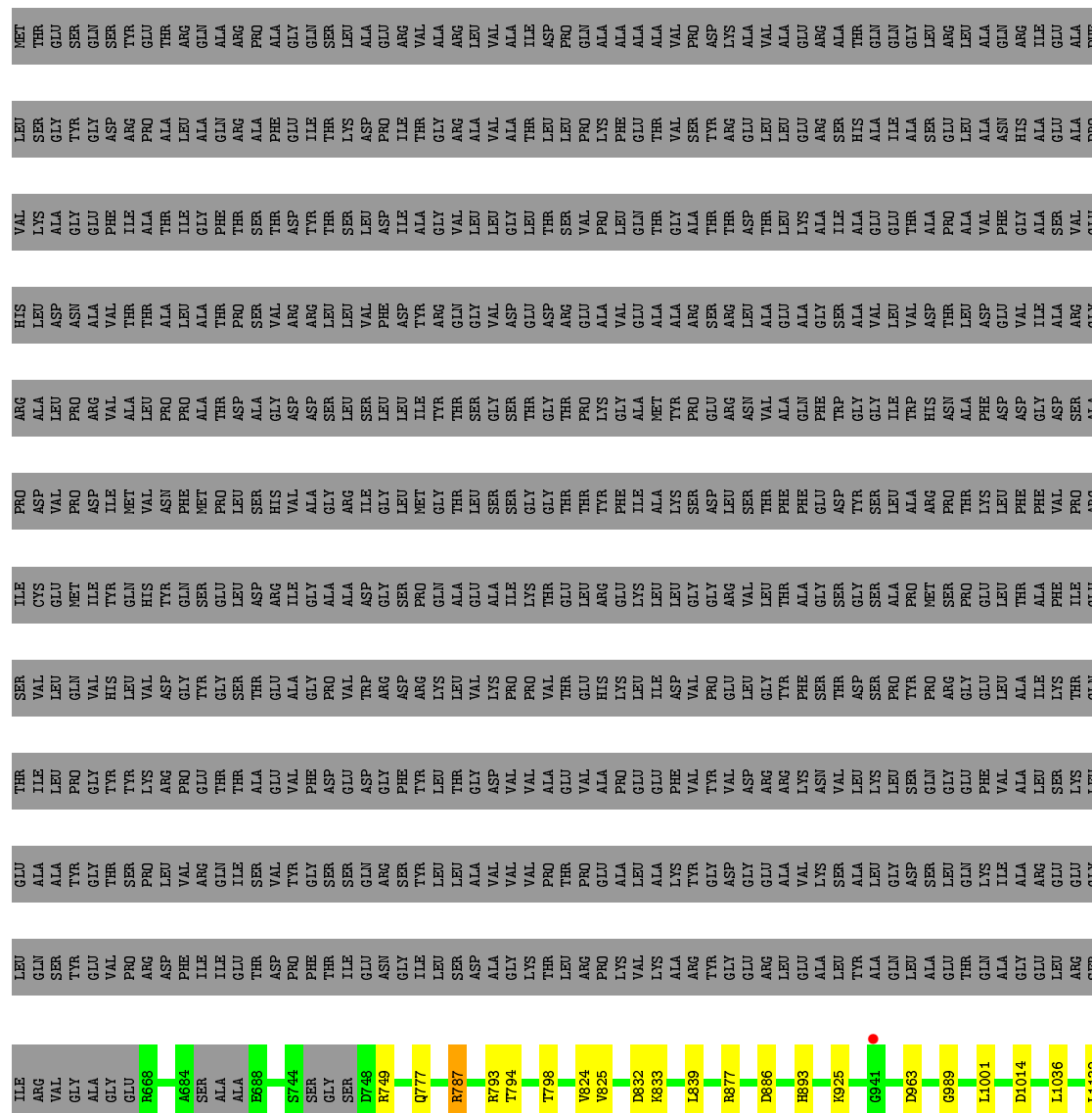
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	208	Total 208	O 208	0	0



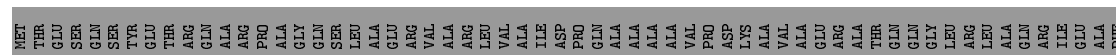
- Molecule 1: Thioester reductase domain-containing protein

Chain B: 41% 1% 57%



- Molecule 1: Thioester reductase domain-containing protein

Chain C:  41% . 57%



ILE	ARG	VAL	GLY	ALA	GLY	PRO	ASP	GLN	THR	SER	ILE	PRO
R668				GLU	THR	THR	ASP	LEU	ARG	VAL	GLN	THR
A694				ASP	VAL	PRO	GLY	GLN	GLY	GLY	GLN	THR
SER				PHE	ILE	ILE	THR	ILE	GLU	GLY	GLY	THR
ALA				ILE	GLN	ILE	THR	ARG	THR	GLY	GLY	THR
ALA				GLU	ILE	GLU	THR	SER	ALA	THR	ASP	THR
V689				THR	ASP	ASP	VAL	VAL	GLU	GLU	ARG	THR
				PRO	THR	THR	TYR	VAL	VAL	GLY	PRO	THR
L782				PHE	THR	SER	GLY	PHE	ASP	PRO	ALA	THR
S744				ILE	SER	SER	ASP	GLU	GLU	VAL	ASP	THR
G746				GLU	GLN	GLN	ASP	ASP	ASP	TRP	ASP	THR
S747				ASN	ARG	ARG	PHE	SER	PHE	ASP	SER	THR
D748				GLY	SER	TYR	TYR	ILE	TYR	ARG	PRO	GLN
				ILE	ILE	LEU	LEU	LEU	THR	LYS	LEU	ALA
E771				SER	SER	LEU	THR	LEU	THR	LEU	ALA	THR
Q777				ASP	ASP	ALA	GLY	GLY	GLU	LYS	ALA	LEU
				ALA	VAL	VAL	VAL	VAL	VAL	PRO	ILE	LYS
R793				GLY	VAL	VAL	VAL	VAL	ALA	VAL	PRO	LYS
T798				LYS	THR	THR	PRO	ALA	ALA	VAL	THR	THR
				LEU	LEU	ARG	THR	THR	VAL	GLU	GLU	THR
V824				ARG	ARG	PRO	PRO	VAL	VAL	GLU	LEU	THR
V825				LYS	GLU	GLU	GLU	ALA	PRO	LYS	ARG	TYR
				VAL	VAL	VAL	LEU	GLU	GLY	LEU	LYS	ILE
L839				LYS	LYS	ALA	ALA	GLY	GLY	ILE	LEU	ALA
				ALA	ALA	LYS	PHE	PHE	ASP	ASP	LYS	LYS
D886				ARG	TYR	TYR	VAL	VAL	VAL	VAL	LEU	LEU
G895				TYR	GLY	GLY	ASP	VAL	VAL	PRO	GLY	GLY
				GLY	GLY	GLY	ASP	ASP	ASP	LEU	VAL	SER
K925				ARG	GLY	ARG	ARG	ARG	ARG	GLY	LEU	THR
				LEU	ALA	ALA	ALA	ALA	ARG	TYR	THR	PHE
D963				GLY	GLY	VAL	VAL	LYS	LYS	PHE	ALA	GLU
D1014				ALA	LYS	LYS	ASN	ASN	VAL	SER	SER	ASP
				LEU	SER	SER	VAL	VAL	THR	THR	GLY	TYR
L1036				TYR	ALA	ALA	LYS	LYS	LYS	ASP	SER	SER
				LEU	LEU	GLY	LEU	LEU	THR	PRO	ALA	LEU
R1042				GLN	GLN	ASP	SER	SER	SER	TYR	PRO	ARG
				LEU	ALA	ALA	ALA	GLN	GLN	PRO	SER	PRO
L1132				GLU	GLY	GLY	GLY	GLY	GLY	ARG	PRO	LYS
V1156				THR	THR	LYS	PHE	PHE	GLY	GLY	GLU	THR
				GLN	ALA	ILE	VAL	VAL	VAL	LEU	LEU	LEU
L1187				ALA	GLY	ALA	ALA	ALA	ALA	ILE	ALA	PHE
LEU				GLU	GLY	GLU	ARG	SER	SER	LYS	PHE	PHE
				LEU	GLY	GLY	GLY	GLY	THR	THR	ILE	PRO
				ARG	SER	GLY	THR	GLN	GLY	GLY	GLY	PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	92.11Å 92.11Å 363.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 2.34 90.88 – 2.34	Depositor EDS
% Data completeness (in resolution range)	95.2 (200.00-2.34) 95.3 (90.88-2.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.191 , 0.207 0.202 , 0.216	Depositor DCC
R_{free} test set	5923 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16781	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: PNS, 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	0.45	0/4018	0.73	8/5467 (0.1%)
1	B	0.44	0/4024	0.70	4/5475 (0.1%)
1	C	0.44	1/4024 (0.0%)	0.70	9/5475 (0.2%)
1	D	0.43	0/4025	0.66	1/5476 (0.0%)
All	All	0.44	1/16091 (0.0%)	0.70	22/21893 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1164	GLU	CG-CD	5.56	1.60	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	963	ASP	CB-CG-OD2	12.93	129.94	118.30
1	A	963	ASP	CB-CG-OD1	-11.32	108.11	118.30
1	A	1101	ARG	CG-CD-NE	10.99	134.87	111.80
1	C	749	ARG	CG-CD-NE	8.96	130.61	111.80
1	B	749	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	C	793	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	1101	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	C	963	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	1101	ARG	CD-NE-CZ	5.89	131.84	123.60
1	A	877	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	963	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	877	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	963	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	960	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	877	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	1150	LYS	CD-CE-NZ	5.54	124.43	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	877	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	877	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	1044	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	1101	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	960	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	C	877	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3932	0	3879	3	0
1	B	3938	0	3881	4	0
1	C	3938	0	3886	6	0
1	D	3939	0	3883	2	0
2	A	21	0	21	0	0
2	B	21	0	21	0	0
2	C	21	0	21	0	0
2	D	21	0	21	0	0
3	A	40	0	19	0	0
3	B	40	0	19	0	0
3	C	40	0	19	0	0
3	D	40	0	19	0	0
4	A	223	0	0	0	0
4	B	195	0	0	0	0
4	C	164	0	0	0	0
4	D	208	0	0	0	0
All	All	16781	0	15689	13	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 0.

All (13) 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:C:960:ARG:HD2	1:C:975:TRP:CD2	2.34	0.62
1:C:1031:LYS:HA	1:C:1101:ARG:HD3	1.84	0.58
1:A:836:LYS:HD2	1:B:833:LYS:HE2	1.87	0.56
1:B:787:ARG:NH2	1:B:989:GLY:O	2.40	0.54
1:B:798:THR:OG1	1:B:893:HIS:HA	2.11	0.51
1:C:749:ARG:NH2	1:C:917:GLU:OE2	2.45	0.49
1:D:798:THR:HG22	1:D:895:GLY:HA3	1.95	0.48
1:C:960:ARG:HD2	1:C:975:TRP:CE2	2.49	0.48
1:A:798:THR:HG22	1:A:895:GLY:HA3	1.96	0.47
1:C:690:ASP:OD1	1:C:692:GLU:N	2.47	0.47
1:A:831:ASP:HB2	1:B:832:ASP:OD2	2.15	0.47
1:C:798:THR:HG22	1:C:895:GLY:HA3	1.97	0.45
1:D:689:VAL:HG12	1:D:732:LEU:CD2	2.49	0.42

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	508/1188 (43%)	496 (98%)	12 (2%)	0	100	100
1	B	508/1188 (43%)	496 (98%)	12 (2%)	0	100	100
1	C	508/1188 (43%)	496 (98%)	12 (2%)	0	100	100
1	D	509/1188 (43%)	496 (97%)	13 (3%)	0	100	100
All	All	2033/4752 (43%)	1984 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	411/947 (43%)	396 (96%)	15 (4%)	40	51
1	B	411/947 (43%)	397 (97%)	14 (3%)	42	53
1	C	412/947 (44%)	398 (97%)	14 (3%)	42	53
1	D	411/947 (43%)	395 (96%)	16 (4%)	37	48
All	All	1645/3788 (43%)	1586 (96%)	59 (4%)	40	51

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	777	GLN
1	A	790	SER
1	A	793	ARG
1	A	824	VAL
1	A	839	LEU
1	A	886	ASP
1	A	925	LYS
1	A	964	GLU
1	A	1001	LEU
1	A	1014	ASP
1	A	1101	ARG
1	A	1132	LEU
1	A	1150	LYS
1	A	1156	VAL
1	A	1188	LEU
1	B	777	GLN
1	B	787	ARG
1	B	793	ARG
1	B	794	THR
1	B	824	VAL
1	B	825	VAL
1	B	839	LEU
1	B	886	ASP
1	B	925	LYS
1	B	1001	LEU
1	B	1014	ASP
1	B	1036	LEU
1	B	1132	LEU

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Mol	Chain	Res	Type
1	B	1156	VAL
1	C	690	ASP
1	C	777	GLN
1	C	793	ARG
1	C	822	LYS
1	C	824	VAL
1	C	825	VAL
1	C	839	LEU
1	C	886	ASP
1	C	925	LYS
1	C	960	ARG
1	C	1014	ASP
1	C	1132	LEU
1	C	1150	LYS
1	C	1156	VAL
1	D	689	VAL
1	D	732	LEU
1	D	748	ASP
1	D	771	GLU
1	D	777	GLN
1	D	793	ARG
1	D	824	VAL
1	D	825	VAL
1	D	839	LEU
1	D	886	ASP
1	D	925	LYS
1	D	1014	ASP
1	D	1036	LEU
1	D	1042	ARG
1	D	1132	LEU
1	D	1156	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	777	GLN
1	C	777	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PNS	A	1201	1	15,20,21	0.57	0	17,26,29	0.94	0
3	NAP	A	1202	-	36,43,52	0.86	1 (2%)	42,67,80	1.47	3 (7%)
2	PNS	B	1201	1	15,20,21	0.57	0	17,26,29	0.87	0
3	NAP	B	1202	-	36,43,52	0.84	1 (2%)	42,67,80	1.45	3 (7%)
2	PNS	C	1201	1	15,20,21	0.64	0	17,26,29	0.83	0
3	NAP	C	1202	-	36,43,52	0.82	1 (2%)	42,67,80	1.54	4 (9%)
2	PNS	D	1201	1	15,20,21	0.57	0	17,26,29	0.88	0
3	NAP	D	1202	-	36,43,52	0.90	1 (2%)	42,67,80	1.57	4 (9%)

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	PNS	A	1201	1	-	0/24/26/27	0/0/0/0
3	NAP	A	1202	-	-	0/23/59/67	0/4/4/5
2	PNS	B	1201	1	-	0/24/26/27	0/0/0/0
3	NAP	B	1202	-	-	0/23/59/67	0/4/4/5
2	PNS	C	1201	1	-	0/24/26/27	0/0/0/0
3	NAP	C	1202	-	-	0/23/59/67	0/4/4/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PNS	D	1201	1	-	0/24/26/27	0/0/0/0
3	NAP	D	1202	-	-	0/23/59/67	0/4/4/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1202	NAP	C5A-C4A	2.61	1.46	1.40
3	C	1202	NAP	C5A-C4A	2.78	1.46	1.40
3	A	1202	NAP	C5A-C4A	2.83	1.46	1.40
3	D	1202	NAP	C5A-C4A	2.84	1.46	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	NAP	N3A-C2A-N1A	-7.62	122.22	128.86
3	D	1202	NAP	N3A-C2A-N1A	-7.15	122.63	128.86
3	A	1202	NAP	N3A-C2A-N1A	-6.93	122.83	128.86
3	B	1202	NAP	N3A-C2A-N1A	-6.63	123.08	128.86
3	D	1202	NAP	C4A-C5A-N7A	-3.10	106.41	109.41
3	B	1202	NAP	C4B-O4B-C1B	-2.97	106.61	109.77
3	D	1202	NAP	C1B-N9A-C4A	-2.83	121.75	126.64
3	D	1202	NAP	C3B-C2B-C1B	-2.74	97.38	102.75
3	C	1202	NAP	C4A-C5A-N7A	-2.54	106.95	109.41
3	C	1202	NAP	C1B-N9A-C4A	-2.27	122.72	126.64
3	A	1202	NAP	C1B-N9A-C4A	-2.13	122.96	126.64
3	A	1202	NAP	C3B-C2B-C1B	-2.01	98.82	102.75
3	B	1202	NAP	C4A-C5A-N7A	-2.00	107.48	109.41
3	C	1202	NAP	C2A-N1A-C6A	2.16	122.54	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	514/1188 (43%)	-0.06	1 (0%) 94 97	15, 40, 71, 106	0
1	B	514/1188 (43%)	0.08	1 (0%) 94 97	18, 44, 76, 107	0
1	C	514/1188 (43%)	0.09	3 (0%) 89 93	21, 47, 76, 100	0
1	D	515/1188 (43%)	-0.01	1 (0%) 94 97	20, 42, 73, 102	0
All	All	2057/4752 (43%)	0.03	6 (0%) 93 97	15, 43, 75, 107	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	946	ALA	3.7
1	C	745	SER	2.3
1	A	745	SER	2.2
1	B	941	GLY	2.1
1	D	746	GLY	2.1
1	C	748	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	PNS	C	1201	21/22	0.97	0.15	0.34	22,27,37,58	0
2	PNS	A	1201	21/22	0.97	0.12	-0.47	19,25,41,60	0
2	PNS	B	1201	21/22	0.95	0.12	-0.62	21,27,39,57	0
3	NAP	C	1202	40/48	0.98	0.11	-0.84	16,20,25,27	0
2	PNS	D	1201	21/22	0.97	0.11	-1.04	20,23,36,55	0
3	NAP	A	1202	40/48	0.99	0.10	-1.33	10,14,20,23	0
3	NAP	B	1202	40/48	0.99	0.09	-1.63	12,15,23,26	0
3	NAP	D	1202	40/48	0.99	0.10	-1.78	14,16,20,20	0

6.5 Other polymers

There are no such residues in this entry.