



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:35 pm GMT

PDB ID : 1VLH  
Title : Crystal structure of Phosphopantetheine adenylyltransferase (TM0741) from *Thermotoga maritima* at 2.20 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2004-07-23  
Resolution : 2.20 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](mailto: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.

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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	:	trunk28620
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)	:	recalc28949

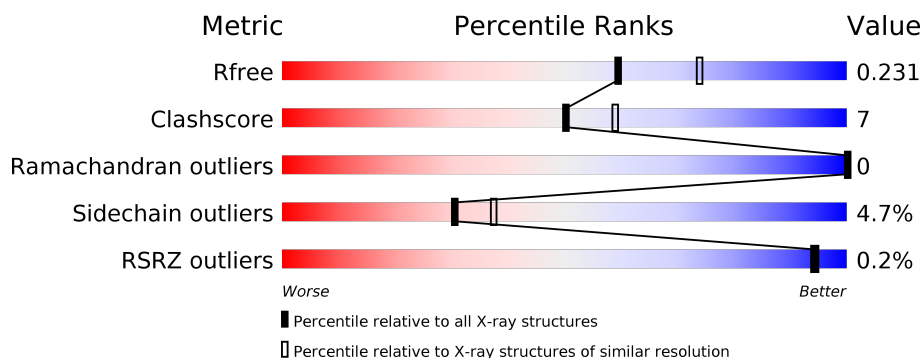
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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  $\geq 3$ , 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	173	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	173	<div> <div>72%</div> <div>17%</div> <div>•</div> <div>9%</div> </div>
1	C	173	<div> <div>72%</div> <div>19%</div> <div>•</div> <div>9%</div> </div>
1	D	173	<div> <div>73%</div> <div>16%</div> <div>••</div> <div>9%</div> </div>
1	E	173	<div> <div>80%</div> <div>10%</div> <div>•</div> <div>9%</div> </div>
1	F	173	<div> <div>%</div> <div>75%</div> <div>14%</div> <div>•</div> <div>9%</div> </div>

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	PNS	A	200	X	-	-	-
2	PNS	B	200	X	-	-	-
2	PNS	C	200	X	-	-	-
2	PNS	D	200	X	-	-	-
2	PNS	E	200	X	-	-	-
2	PNS	F	200	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7933 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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	2	0
			1262	820	205	232	5			
1	B	158	Total	C	N	O	S	0	0	0
			1256	816	203	233	4			
1	C	158	Total	C	N	O	S	0	0	0
			1261	819	205	233	4			
1	D	158	Total	C	N	O	S	0	0	0
			1255	815	203	233	4			
1	E	157	Total	C	N	O	S	0	0	0
			1251	814	203	230	4			
1	F	157	Total	C	N	O	S	0	0	0
			1250	813	203	230	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9WZK0
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZK0
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WZK0
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZK0
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZK0
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZK0
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
B	-11	MET	-	LEADER SEQUENCE	UNP Q9WZK0
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZK0
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WZK0
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZK0
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZK0

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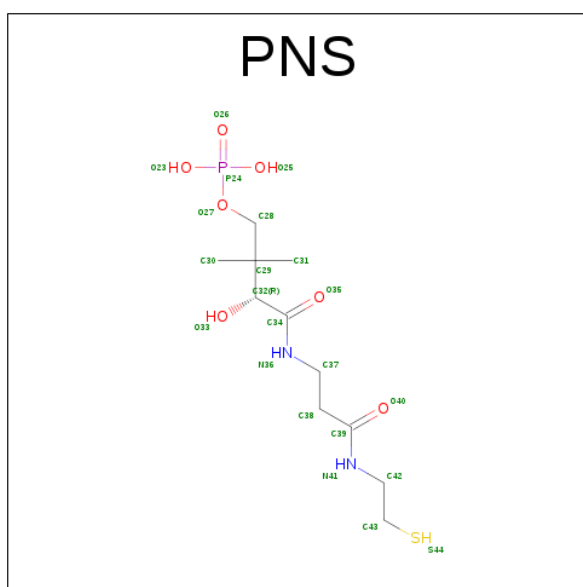
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZK0
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WZK0
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZK0
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WZK0
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZK0
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZK0
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZK0
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
D	-11	MET	-	LEADER SEQUENCE	UNP Q9WZK0
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZK0
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WZK0
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZK0
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZK0
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZK0
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
E	-11	MET	-	LEADER SEQUENCE	UNP Q9WZK0
E	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZK0
E	-9	SER	-	LEADER SEQUENCE	UNP Q9WZK0
E	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZK0
E	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZK0
E	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZK0
E	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
E	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
E	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
E	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
E	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZK0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
F	-11	MET	-	LEADER SEQUENCE	UNP Q9WZK0
F	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZK0
F	-9	SER	-	LEADER SEQUENCE	UNP Q9WZK0
F	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZK0
F	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZK0
F	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZK0
F	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
F	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
F	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
F	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
F	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZK0
F	0	HIS	-	LEADER SEQUENCE	UNP Q9WZK0

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula:  $C_{11}H_{23}N_2O_7PS$ ).



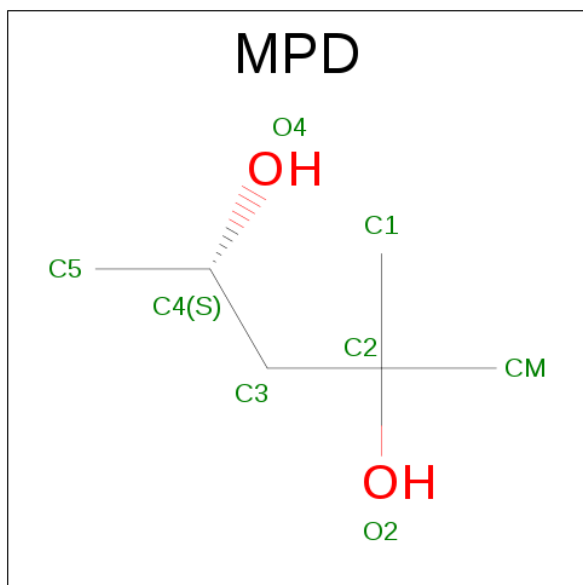
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 22	C 11	N 2	O 7	P 1	S 1	0	0
2	B	1	Total 22	C 11	N 2	O 7	P 1	S 1	0	0
2	C	1	Total 22	C 11	N 2	O 7	P 1	S 1	0	0
2	D	1	Total 22	C 11	N 2	O 7	P 1	S 1	0	0
2	E	1	Total 22	C 11	N 2	O 7	P 1	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	S	
			22	11	2	7	1	1	
								0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O		
			8	6	2	0	0

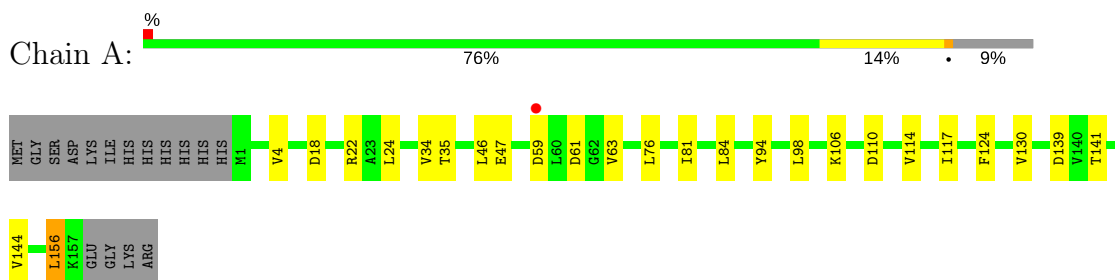
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O		
			39	39	0	0
4	B	50	Total	O		
			50	50	0	0
4	C	37	Total	O		
			37	37	0	0
4	D	45	Total	O		
			45	45	0	0
4	E	44	Total	O		
			44	44	0	0
4	F	43	Total	O		
			43	43	0	0

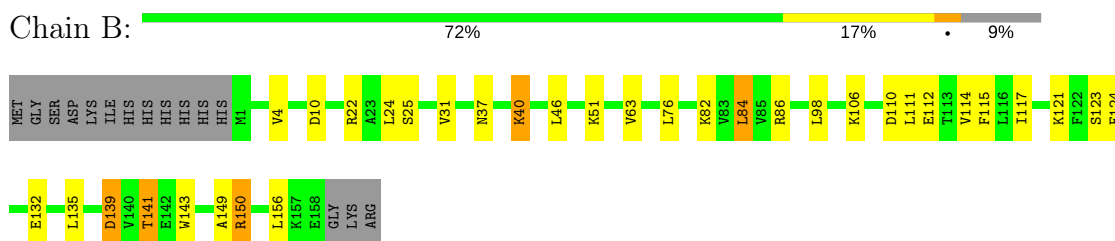
### 3 Residue-property plots [i](#)

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.

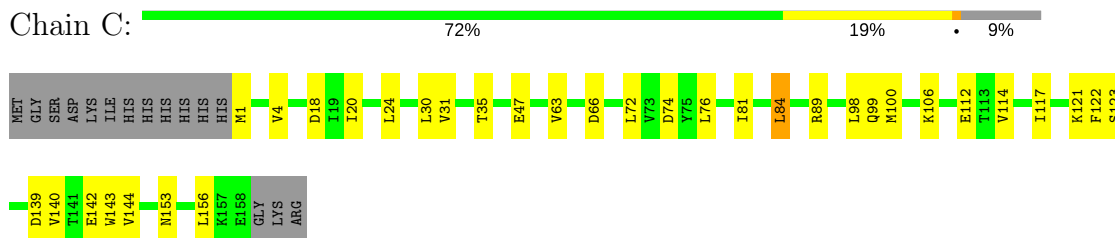
- Molecule 1: Phosphopantetheine adenylyltransferase



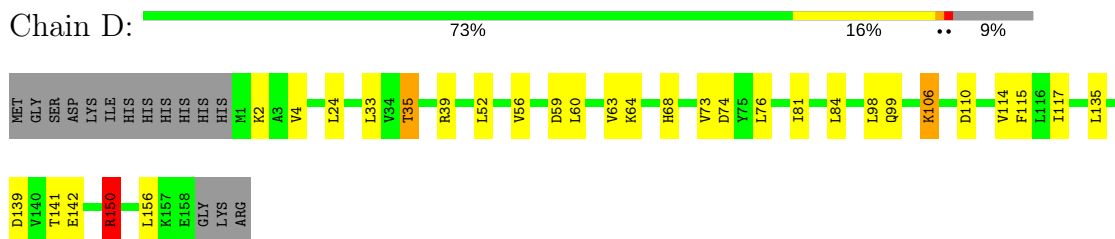
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase

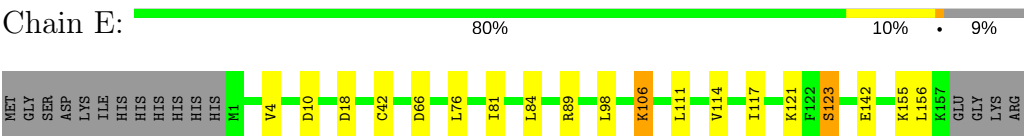


- Molecule 1: Phosphopantetheine adenylyltransferase

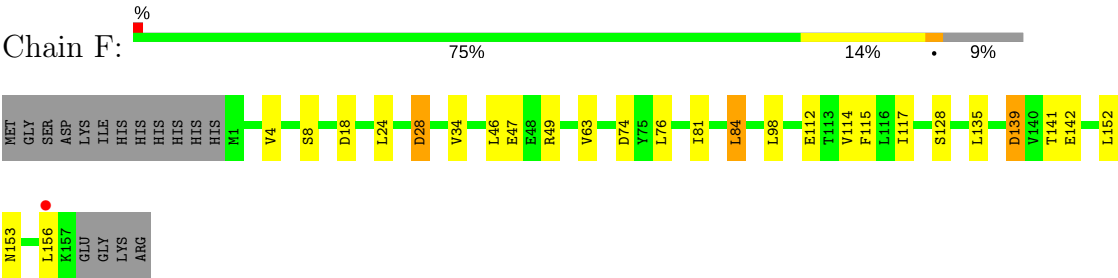




● Molecule 1: Phosphopantetheine adenylyltransferase



● Molecule 1: Phosphopantetheine adenylyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.96Å 110.88Å 74.09Å 90.00° 111.98° 90.00°	Depositor
Resolution (Å)	68.70 – 2.20 68.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (68.70-2.20) 94.4 (68.70-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.171 , 0.227 0.179 , 0.231	Depositor DCC
$R_{free}$ test set	2497 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.79	0/1284	0.89	4/1734 (0.2%)
1	B	0.76	0/1278	0.91	4/1727 (0.2%)
1	C	0.71	0/1283	0.89	4/1732 (0.2%)
1	D	0.78	1/1277 (0.1%)	0.88	4/1726 (0.2%)
1	E	0.76	0/1273	0.88	3/1719 (0.2%)
1	F	0.74	0/1272	0.86	4/1718 (0.2%)
All	All	0.76	1/7667 (0.0%)	0.89	23/10356 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	VAL	CB-CG1	-5.20	1.42	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	150	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	F	18	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	10	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	18	ASP	CB-CG-OD2	6.03	123.73	118.30
1	D	110	ASP	CB-CG-OD2	5.87	123.59	118.30
1	B	150	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	61	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	59	ASP	CB-CG-OD2	5.82	123.53	118.30
1	F	28	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	139	ASP	CB-CG-OD2	5.75	123.48	118.30
1	E	18	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	22	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	C	66	ASP	CB-CG-OD2	5.51	123.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	74	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	139	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	59	ASP	CB-CG-OD2	5.39	123.15	118.30
1	F	74	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	139	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	10	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	74	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	66	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1262	0	1308	21	0
1	B	1256	0	1298	24	0
1	C	1261	0	1314	20	0
1	D	1255	0	1296	27	0
1	E	1251	0	1303	15	0
1	F	1250	0	1301	18	0
2	A	22	0	21	1	0
2	B	22	0	20	0	0
2	C	22	0	21	1	0
2	D	22	0	20	0	0
2	E	22	0	21	4	0
2	F	22	0	21	1	0
3	B	8	0	14	1	0
4	A	39	0	0	2	0
4	B	50	0	0	0	0
4	C	37	0	0	2	0
4	D	45	0	0	0	0
4	E	44	0	0	2	0
4	F	43	0	0	0	0
All	All	7933	0	7958	103	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 7.

All (103) 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)
2:E:200:PNS:H313	2:E:200:PNS:H36	1.33	0.94
1:D:114:VAL:HG13	1:E:114:VAL:HG13	1.49	0.92
2:E:200:PNS:H313	2:E:200:PNS:N36	1.84	0.91
1:E:76:LEU:HD21	1:E:84:LEU:HD13	1.54	0.89
1:A:114:VAL:HG13	1:B:114:VAL:HG13	1.53	0.88
1:F:76:LEU:HD21	1:F:84:LEU:HD13	1.59	0.84
1:F:152:LEU:O	1:F:156:LEU:HG	1.79	0.83
1:B:143:TRP:CZ2	1:D:106:LYS:HG2	2.16	0.81
1:D:4:VAL:HG23	1:D:81:ILE:HG21	1.64	0.81
1:B:139:ASP:OD1	1:B:141:THR:HB	1.82	0.79
1:D:76:LEU:HD11	1:D:84:LEU:HD13	1.67	0.74
1:B:143:TRP:HZ2	1:D:106:LYS:HG2	1.53	0.71
1:A:98:LEU:HD22	1:B:117:ILE:HD12	1.72	0.71
1:B:24:LEU:HD11	1:B:63:VAL:CG2	2.21	0.70
1:B:76:LEU:HD21	1:B:84:LEU:HD13	1.75	0.68
1:F:24:LEU:HD11	1:F:63:VAL:HG22	1.74	0.68
1:E:42:CYS:HB3	4:E:234:HOH:O	1.93	0.68
1:C:114:VAL:HG13	1:F:114:VAL:HG13	1.75	0.68
1:A:34:VAL:HG12	1:A:46:LEU:HD23	1.74	0.67
1:C:76:LEU:HD21	1:C:84:LEU:HD13	1.77	0.66
1:D:139:ASP:OD1	1:D:141:THR:HB	1.95	0.66
1:C:98:LEU:HD22	1:F:117:ILE:HD12	1.77	0.66
1:A:24:LEU:HD11	1:A:63:VAL:CG2	2.26	0.65
1:C:24:LEU:HD11	1:C:63:VAL:CG2	2.26	0.65
1:F:135:LEU:HA	1:F:156:LEU:HD13	1.80	0.64
1:B:4:VAL:HG22	1:B:31:VAL:HB	1.79	0.64
1:F:135:LEU:CD2	1:F:156:LEU:HD22	2.27	0.63
1:A:114:VAL:HG13	1:B:114:VAL:CG1	2.26	0.63
1:D:150:ARG:HH11	1:D:150:ARG:HG3	1.65	0.62
1:A:117:ILE:HD12	1:B:98:LEU:CD1	2.31	0.61
1:A:156:LEU:HD12	1:A:156:LEU:O	2.00	0.61
1:A:76:LEU:HD21	1:A:84:LEU:HD13	1.82	0.60
1:A:117:ILE:HD12	1:B:98:LEU:HD12	1.83	0.59
1:C:117:ILE:HD12	1:F:98:LEU:CD2	2.33	0.59
1:D:115:PHE:CE1	1:E:117:ILE:HD11	2.37	0.59
1:F:24:LEU:HD11	1:F:63:VAL:CG2	2.33	0.58
1:B:37:ASN:ND2	1:B:40:LYS:HE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:NE	4:A:237:HOH:O	2.36	0.57
1:A:35:THR:HB	2:A:200:PNS:H313	1.86	0.56
1:B:24:LEU:HD11	1:B:63:VAL:HG23	1.86	0.56
1:C:143:TRP:CZ2	1:E:106:LYS:HG2	2.41	0.56
1:F:135:LEU:HD21	1:F:156:LEU:HD22	1.86	0.55
1:A:130:VAL:HG11	1:A:144:VAL:HG11	1.89	0.55
1:E:4:VAL:HG23	1:E:81:ILE:HG21	1.88	0.55
1:B:37:ASN:HB3	1:B:40:LYS:HG3	1.90	0.53
1:C:20:ILE:HG23	1:C:30:LEU:HD23	1.90	0.52
1:C:100:MET:CE	4:C:236:HOH:O	2.58	0.52
1:D:150:ARG:HH11	1:D:150:ARG:CG	2.22	0.52
1:D:114:VAL:CG1	1:E:114:VAL:HG13	2.30	0.52
1:C:121:LYS:HE3	1:C:122:PHE:CZ	2.46	0.51
1:D:4:VAL:HG21	1:D:76:LEU:CD2	2.39	0.51
1:C:117:ILE:HD12	1:F:98:LEU:HD22	1.91	0.51
1:C:72:LEU:N	2:C:200:PNS:O40	2.35	0.51
1:D:33:LEU:O	1:D:35:THR:HG22	2.11	0.51
1:A:98:LEU:CD2	1:B:117:ILE:HD12	2.40	0.50
1:C:140:VAL:O	1:C:144:VAL:HG22	2.12	0.50
1:D:24:LEU:HD11	1:D:63:VAL:CG2	2.41	0.50
1:C:98:LEU:CD2	1:F:117:ILE:HD12	2.42	0.50
1:D:76:LEU:HD11	1:D:84:LEU:CD1	2.42	0.49
1:B:135:LEU:HA	1:B:156:LEU:HD13	1.95	0.48
1:D:33:LEU:HD11	1:D:68:HIS:HB2	1.95	0.48
1:C:4:VAL:HG22	1:C:31:VAL:HB	1.96	0.47
1:D:4:VAL:HG21	1:D:76:LEU:HD23	1.95	0.47
1:A:22:ARG:CZ	4:A:237:HOH:O	2.62	0.47
2:E:200:PNS:H36	2:E:200:PNS:C31	2.11	0.47
1:A:4:VAL:HG23	1:A:81:ILE:HG21	1.96	0.47
1:A:94:TYR:CE1	1:A:98:LEU:HD21	2.50	0.47
1:D:98:LEU:CD2	1:E:117:ILE:HD12	2.44	0.47
1:E:76:LEU:HD23	1:E:111:LEU:HD13	1.94	0.47
1:F:4:VAL:HG23	1:F:81:ILE:HG21	1.97	0.47
1:A:24:LEU:HD11	1:A:63:VAL:HG22	1.96	0.46
1:B:106:LYS:CD	1:F:142:GLU:OE2	2.64	0.46
1:B:37:ASN:HD22	1:B:40:LYS:HE2	1.78	0.46
1:D:139:ASP:OD1	1:D:141:THR:CB	2.63	0.46
1:B:124:PHE:O	1:D:99:GLN:HG3	2.15	0.46
1:A:124:PHE:O	1:C:99:GLN:HG3	2.16	0.46
1:E:89:ARG:HB3	1:E:123:SER:O	2.16	0.46
1:C:4:VAL:HG23	1:C:81:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LEU:O	1:D:56:VAL:HG23	2.15	0.46
1:B:82:LYS:HD3	1:B:110:ASP:HB3	1.97	0.46
2:F:200:PNS:H303	2:F:200:PNS:H36	1.81	0.46
1:E:155:LYS:NZ	4:E:214:HOH:O	2.49	0.45
1:B:76:LEU:HD23	1:B:111:LEU:HD13	2.00	0.44
1:F:139:ASP:OD1	1:F:141:THR:HG23	2.17	0.43
1:A:106[A]:LYS:HD2	1:E:142:GLU:OE1	2.18	0.43
1:C:89:ARG:HB3	1:C:123:SER:O	2.18	0.43
1:C:117:ILE:HD11	1:F:115:PHE:CE1	2.53	0.43
1:D:76:LEU:CD1	1:D:84:LEU:HD13	2.44	0.43
1:B:132:GLU:OE1	1:D:39:ARG:CZ	2.67	0.43
1:C:20:ILE:HG23	1:C:30:LEU:CD2	2.48	0.43
4:C:237:HOH:O	2:E:200:PNS:H311	2.19	0.43
1:B:149:ALA:HB1	3:B:201:MPD:HM2	2.01	0.42
1:D:60:LEU:HD23	1:D:60:LEU:HA	1.90	0.42
1:A:4:VAL:HG23	1:A:81:ILE:HD13	2.01	0.42
1:A:139:ASP:OD1	1:A:141:THR:HB	2.20	0.41
1:F:8:SER:O	1:F:49:ARG:HD2	2.20	0.41
1:D:117:ILE:HD12	1:E:98:LEU:CD1	2.50	0.41
1:F:34:VAL:HG12	1:F:46:LEU:CD2	2.50	0.41
1:D:150:ARG:NH1	1:D:150:ARG:CG	2.82	0.41
1:B:86:ARG:HB2	1:B:115:PHE:CD2	2.55	0.41
1:C:76:LEU:CD2	1:C:84:LEU:HD13	2.49	0.41
1:D:98:LEU:HD22	1:E:117:ILE:HG23	2.03	0.41
1:D:98:LEU:HD23	1:E:117:ILE:HD12	2.02	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	157/173 (91%)	153 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	156/173 (90%)	155 (99%)	1 (1%)	0	100	100
1	C	156/173 (90%)	154 (99%)	2 (1%)	0	100	100
1	D	156/173 (90%)	155 (99%)	1 (1%)	0	100	100
1	E	155/173 (90%)	154 (99%)	1 (1%)	0	100	100
1	F	155/173 (90%)	153 (99%)	2 (1%)	0	100	100
All	All	935/1038 (90%)	924 (99%)	11 (1%)	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	140/154 (91%)	138 (99%)	2 (1%)	71	84
1	B	139/154 (90%)	129 (93%)	10 (7%)	17	18
1	C	141/154 (92%)	132 (94%)	9 (6%)	20	23
1	D	139/154 (90%)	131 (94%)	8 (6%)	23	27
1	E	139/154 (90%)	135 (97%)	4 (3%)	48	60
1	F	139/154 (90%)	133 (96%)	6 (4%)	33	41
All	All	837/924 (91%)	798 (95%)	39 (5%)	30	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	156	LEU
1	B	25	SER
1	B	40	LYS
1	B	46	LEU
1	B	51	LYS
1	B	84	LEU
1	B	112	GLU

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Mol	Chain	Res	Type
1	B	121	LYS
1	B	123	SER
1	B	141	THR
1	B	150	ARG
1	C	1	MET
1	C	35	THR
1	C	47	GLU
1	C	84	LEU
1	C	106	LYS
1	C	112	GLU
1	C	142	GLU
1	C	153	ASN
1	C	156	LEU
1	D	2	LYS
1	D	35	THR
1	D	64	LYS
1	D	106	LYS
1	D	135	LEU
1	D	142	GLU
1	D	150	ARG
1	D	156	LEU
1	E	106	LYS
1	E	121	LYS
1	E	123	SER
1	E	156	LEU
1	F	28	ASP
1	F	47	GLU
1	F	84	LEU
1	F	112	GLU
1	F	128	SER
1	F	153	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	200	-	19,21,21	0.79	0	24,29,29	3.32	9 (37%)
2	PNS	B	200	-	19,21,21	0.84	0	24,29,29	2.64	9 (37%)
3	MPD	B	201	-	7,7,7	0.63	0	9,10,10	0.68	0
2	PNS	C	200	-	19,21,21	0.72	0	24,29,29	2.45	9 (37%)
2	PNS	D	200	-	19,21,21	0.69	0	24,29,29	3.49	10 (41%)
2	PNS	E	200	-	19,21,21	1.10	1 (5%)	24,29,29	2.74	12 (50%)
2	PNS	F	200	-	19,21,21	0.93	1 (5%)	24,29,29	4.18	16 (66%)

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	200	-	1/1/5/7	0/27/27/27	0/0/0/0
2	PNS	B	200	-	1/1/5/7	1/27/27/27	0/0/0/0
3	MPD	B	201	-	-	0/5/5/5	0/0/0/0
2	PNS	C	200	-	1/1/5/7	0/27/27/27	0/0/0/0
2	PNS	D	200	-	1/1/5/7	0/27/27/27	0/0/0/0
2	PNS	E	200	-	1/1/5/7	1/27/27/27	0/0/0/0
2	PNS	F	200	-	1/1/5/7	1/27/27/27	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	200	PNS	C28-C29	2.22	1.55	1.52
2	E	200	PNS	O33-C32	2.98	1.48	1.42

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	200	PNS	C43-C42-N41	-6.97	97.33	112.50
2	A	200	PNS	C32-C34-N36	-6.31	103.45	116.58
2	F	200	PNS	C31-C29-C32	-6.01	98.40	108.82
2	B	200	PNS	O35-C34-N36	-5.80	111.90	123.07
2	F	200	PNS	C30-C29-C28	-5.52	100.25	108.37
2	D	200	PNS	C31-C29-C32	-4.99	100.17	108.82
2	B	200	PNS	C38-C37-N36	-4.60	102.34	111.87
2	C	200	PNS	C43-C42-N41	-4.49	102.73	112.50
2	D	200	PNS	O40-C39-N41	-4.47	114.44	122.97
2	A	200	PNS	C31-C29-C32	-4.20	101.55	108.82
2	E	200	PNS	C38-C39-N41	-4.13	109.36	116.49
2	F	200	PNS	O25-P24-O27	-4.04	95.99	106.73
2	F	200	PNS	O33-C32-C29	-3.97	100.90	110.25
2	F	200	PNS	C38-C39-N41	-3.96	109.66	116.49
2	C	200	PNS	C31-C29-C32	-3.77	102.28	108.82
2	C	200	PNS	O40-C39-N41	-3.75	115.82	122.97
2	E	200	PNS	C43-C42-N41	-3.72	104.41	112.50
2	D	200	PNS	C32-C34-N36	-3.72	108.85	116.58
2	A	200	PNS	O40-C39-C38	-3.33	115.75	122.01
2	F	200	PNS	C43-C42-N41	-3.31	105.31	112.50
2	B	200	PNS	C31-C29-C32	-2.98	103.66	108.82
2	E	200	PNS	C31-C29-C32	-2.92	103.76	108.82
2	E	200	PNS	O33-C32-C29	-2.85	103.54	110.25
2	A	200	PNS	O25-P24-O27	-2.73	99.46	106.73
2	D	200	PNS	C38-C37-N36	-2.41	106.89	111.87
2	C	200	PNS	C32-C34-N36	-2.06	112.29	116.58
2	D	200	PNS	O27-P24-O26	-2.05	100.71	106.47
2	E	200	PNS	O23-P24-O27	-2.05	101.28	106.73
2	B	200	PNS	O23-P24-O26	2.06	118.58	110.50
2	B	200	PNS	P24-O27-C28	2.28	124.59	118.30
2	F	200	PNS	O40-C39-C38	2.40	126.52	122.01
2	B	200	PNS	C37-C38-C39	2.68	116.52	112.22
2	E	200	PNS	C32-C34-N36	2.71	122.22	116.58
2	B	200	PNS	C42-N41-C39	2.84	128.30	122.84
2	C	200	PNS	P24-O27-C28	2.99	126.54	118.30
2	E	200	PNS	O40-C39-N41	3.00	128.71	122.97
2	E	200	PNS	C38-C37-N36	3.08	118.25	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	200	PNS	O27-P24-O26	3.23	115.52	106.47
2	E	200	PNS	C31-C29-C28	3.24	113.13	108.37
2	C	200	PNS	C38-C39-N41	3.33	122.24	116.49
2	F	200	PNS	O27-C28-C29	3.65	116.41	110.55
2	C	200	PNS	C30-C29-C32	3.67	115.19	108.82
2	D	200	PNS	C38-C39-N41	3.72	122.90	116.49
2	F	200	PNS	C42-N41-C39	3.75	130.04	122.84
2	F	200	PNS	C37-C38-C39	3.83	118.38	112.22
2	A	200	PNS	O35-C34-N36	3.83	130.44	123.07
2	A	200	PNS	C30-C29-C32	3.87	115.52	108.82
2	B	200	PNS	C30-C29-C32	3.99	115.73	108.82
2	F	200	PNS	P24-O27-C28	4.00	129.31	118.30
2	E	200	PNS	O27-C28-C29	4.00	116.98	110.55
2	A	200	PNS	C37-C38-C39	4.04	118.72	112.22
2	A	200	PNS	C38-C39-N41	4.18	123.69	116.49
2	E	200	PNS	C42-N41-C39	4.56	131.59	122.84
2	C	200	PNS	C37-N36-C34	4.61	131.19	122.59
2	F	200	PNS	C32-C34-N36	4.70	126.37	116.58
2	F	200	PNS	C38-C37-N36	4.85	121.91	111.87
2	D	200	PNS	C37-N36-C34	4.94	131.79	122.59
2	C	200	PNS	C42-N41-C39	5.00	132.45	122.84
2	F	200	PNS	C30-C29-C32	5.23	117.89	108.82
2	E	200	PNS	C37-N36-C34	6.41	134.54	122.59
2	B	200	PNS	C37-N36-C34	6.72	135.12	122.59
2	D	200	PNS	C30-C29-C32	6.92	120.82	108.82
2	D	200	PNS	C42-N41-C39	8.66	139.47	122.84
2	A	200	PNS	C37-N36-C34	10.51	142.18	122.59
2	F	200	PNS	C31-C29-C28	11.40	125.12	108.37

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	200	PNS	C32
2	D	200	PNS	C32
2	A	200	PNS	C32
2	E	200	PNS	C32
2	C	200	PNS	C32
2	B	200	PNS	C32

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	200	PNS	O35-C34-C32-C29
2	F	200	PNS	O35-C34-C32-C29
2	B	200	PNS	C32-C34-N36-C37

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	PNS	1	0
3	B	201	MPD	1	0
2	C	200	PNS	1	0
2	E	200	PNS	4	0
2	F	200	PNS	1	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	157/173 (90%)	-0.13	1 (0%) 89 88	34, 43, 55, 65	0
1	B	158/173 (91%)	-0.18	0 100 100	34, 42, 55, 64	1 (0%)
1	C	158/173 (91%)	-0.19	0 100 100	34, 43, 56, 65	0
1	D	158/173 (91%)	-0.11	0 100 100	34, 43, 55, 66	2 (1%)
1	E	157/173 (90%)	-0.19	0 100 100	34, 42, 55, 66	0
1	F	157/173 (90%)	-0.24	1 (0%) 89 88	34, 43, 54, 63	3 (1%)
All	All	945/1038 (91%)	-0.17	2 (0%) 94 94	34, 43, 55, 66	6 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ASP	4.8
1	F	156	LEU	3.1

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	PNS	F	200	22/22	0.94	0.14	1.58	46,55,62,66	0
2	PNS	C	200	22/22	0.96	0.16	1.38	39,52,59,60	0
2	PNS	A	200	22/22	0.96	0.15	0.80	37,50,58,61	0
2	PNS	E	200	22/22	0.94	0.15	0.65	33,48,55,59	0
2	PNS	B	200	22/22	0.95	0.12	-0.01	40,46,57,61	0
2	PNS	D	200	22/22	0.96	0.12	-0.59	38,48,56,57	0
3	MPD	B	201	8/8	0.96	0.10	-1.05	34,41,47,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.