



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:57 PM GMT

PDB ID : 4NAH  
Title : Inhibitors of 4-Phosphopanthetheine Adenylyltransferase (PPAT)  
Authors : Lahiri, S.D.  
Deposited on : 2013-10-22  
Resolution : 2.38 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

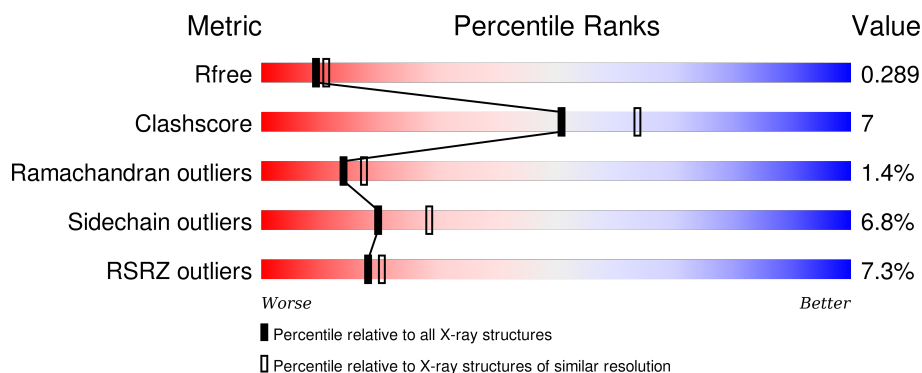
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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))
$R_{free}$	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	160	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	B	160	<div> <div>9%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	C	160	<div> <div>7%</div> <div>84%</div> <div>13%</div> <div>• •</div> </div>
1	D	160	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>• • •</div> </div>
1	E	160	<div> <div>12%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	160	<div><div></div><div>10%</div><div></div><div>87%</div><div></div><div>12%</div><div>..</div></div>

## 2 Entry composition [i](#)

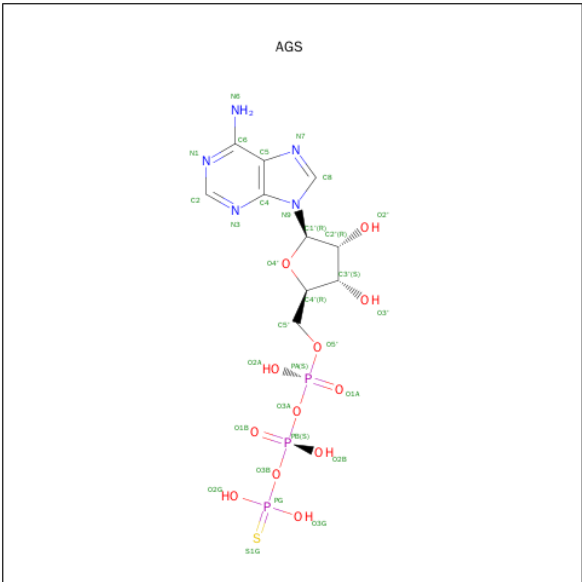
There are 4 unique types of molecules in this entry. The entry contains 8204 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

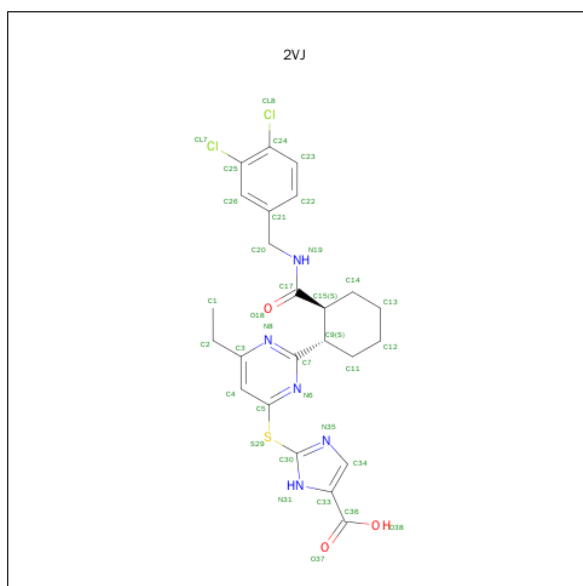
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	1	0
			1285	821	213	244	7			
1	B	160	Total	C	N	O	S	0	0	0
			1290	824	214	245	7			
1	C	160	Total	C	N	O	S	0	0	0
			1290	824	214	245	7			
1	D	159	Total	C	N	O	S	0	1	0
			1285	821	213	244	7			
1	E	160	Total	C	N	O	S	0	0	0
			1290	824	214	245	7			
1	F	160	Total	C	N	O	S	0	0	0
			1290	824	214	245	7			

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is 2-[(2-{(1S,2S)-2-[(3,4-DICHLOROBENZYL)CARBAMOYL]CYCLOHEXYL}-6-ETHYLPYRIMIDIN-4-YL)SULFANYL]-1H-IMIDAZOLE-5-CARBOXYLIC ACID (three-letter code: 2VJ) (formula: C<sub>24</sub>H<sub>25</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			35	24	2	5	3	1		
3	A	1	Total	C	Cl	N	O	S	0	0
			35	24	2	5	3	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			35	24	2	5	3	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			35	24	2	5	3	1		
3	F	1	Total	C	Cl	N	O	S	0	0
			35	24	2	5	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	Cl	N	O	S	
			35	24	2	5	3	1	
								0	0

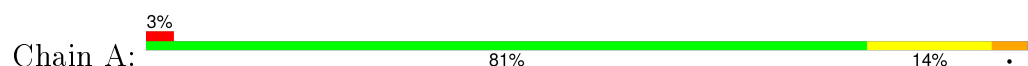
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O		
			17	17	0	0
4	B	22	Total	O		
			22	22	0	0
4	C	13	Total	O		
			13	13	0	0
4	D	10	Total	O		
			10	10	0	0
4	E	3	Total	O		
			3	3	0	0
4	F	13	Total	O		
			13	13	0	0

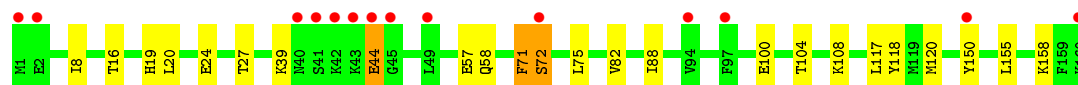
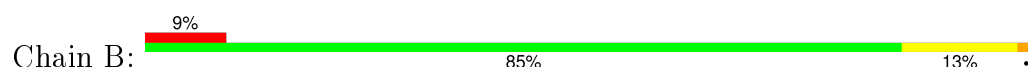
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

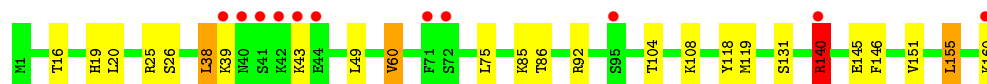
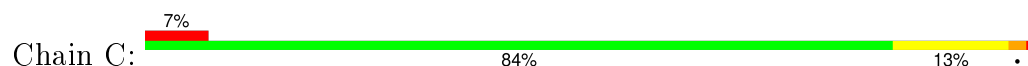
- Molecule 1: Phosphopantetheine adenylyltransferase



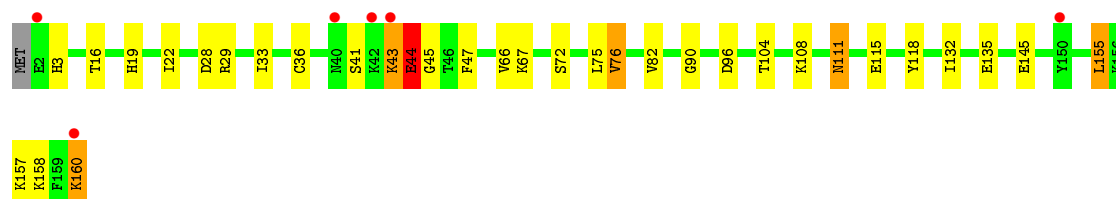
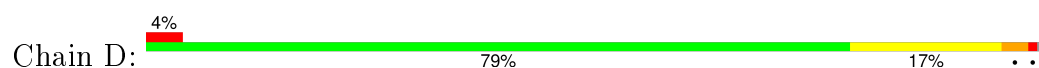
- Molecule 1: Phosphopantetheine adenylyltransferase



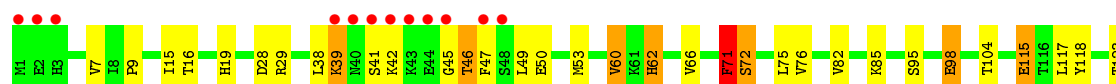
- Molecule 1: Phosphopantetheine adenylyltransferase

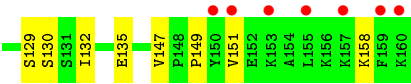


- Molecule 1: Phosphopantetheine adenylyltransferase

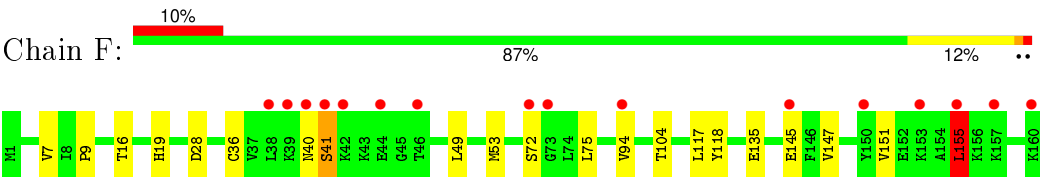


- Molecule 1: Phosphopantetheine adenylyltransferase





● Molecule 1: Phosphopantetheine adenylyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.48 Å 105.36 Å 79.98 Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	41.70 – 2.38 41.70 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.70-2.38) 99.1 (41.70-2.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.93 (at 2.37 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.216 , 0.292 0.221 , 0.289	Depositor DCC
$R_{free}$ test set	2275 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 45151 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 2VJ, AGS

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	0.75	0/1312	0.83	0/1767
1	B	0.78	0/1314	0.87	0/1769
1	C	0.72	0/1314	0.82	2/1769 (0.1%)
1	D	0.79	0/1312	0.86	3/1767 (0.2%)
1	E	0.72	0/1314	0.84	1/1769 (0.1%)
1	F	0.68	0/1314	0.80	1/1769 (0.1%)
All	All	0.74	0/7880	0.84	7/10610 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	155	LEU	CA-CB-CG	7.40	132.33	115.30
1	D	36[A]	CYS	N-CA-CB	-6.30	99.26	110.60
1	D	36[B]	CYS	N-CA-CB	-6.30	99.26	110.60
1	C	25	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	E	71	PHE	C-N-CA	5.51	135.47	121.70
1	D	96	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	140	ARG	NE-CZ-NH1	5.39	122.99	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	71	PHE	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1285	0	1297	22	0
1	B	1290	0	1304	18	0
1	C	1290	0	1304	16	0
1	D	1285	0	1297	18	0
1	E	1290	0	1304	24	0
1	F	1290	0	1304	13	0
2	A	31	0	12	4	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	3	0
2	E	31	0	12	0	0
2	F	31	0	12	1	0
3	A	70	0	49	6	0
3	B	35	0	25	1	0
3	D	35	0	25	3	0
3	F	70	0	49	2	0
4	A	17	0	0	2	0
4	B	22	0	0	1	0
4	C	13	0	0	1	0
4	D	10	0	0	1	0
4	E	3	0	0	0	0
4	F	13	0	0	0	0
All	All	8204	0	8030	111	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 (111) 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:E:115:GLU:OE2	1:E:117:LEU:HD13	1.42	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLU:HB2	1:D:45:GLY:O	1.66	0.96
1:C:38:LEU:HD12	1:C:38:LEU:H	1.42	0.83
1:B:104:THR:HG21	1:B:118:TYR:OH	1.80	0.81
2:D:201:AGS:O2B	2:D:201:AGS:O3G	2.01	0.78
1:A:36[B]:CYS:SG	3:A:203:2VJ:CL7	2.79	0.78
1:C:140:ARG:HH11	1:C:140:ARG:HB2	1.49	0.77
1:A:104:THR:OG1	1:A:118:TYR:OH	2.04	0.76
2:A:201:AGS:O1B	4:A:313:HOH:O	2.05	0.74
1:E:115:GLU:OE2	1:E:117:LEU:CD1	2.30	0.74
1:B:71:PHE:CG	1:B:72:SER:HB2	2.23	0.74
1:E:38:LEU:HD23	1:E:39:LYS:N	2.04	0.73
2:A:201:AGS:O2B	2:A:201:AGS:S1G	2.47	0.73
1:E:9:PRO:HG3	1:E:75:LEU:HD21	1.72	0.72
1:A:7:VAL:HG13	1:A:36[A]:CYS:SG	2.31	0.71
1:C:140:ARG:NH1	1:C:140:ARG:HB2	2.05	0.71
1:E:50:GLU:OE1	1:E:50:GLU:N	2.24	0.70
1:B:104:THR:HG22	4:B:302:HOH:O	1.91	0.69
1:C:104:THR:OG1	1:C:118:TYR:OH	2.09	0.69
1:A:135:GLU:OE2	3:A:202:2VJ:C34	2.39	0.69
1:F:151:VAL:O	1:F:155:LEU:HD23	1.92	0.69
2:A:201:AGS:O2B	3:A:203:2VJ:O38	2.13	0.67
1:B:71:PHE:HA	1:B:72:SER:HB2	1.76	0.66
1:F:16:THR:HA	1:F:147:VAL:HG12	1.79	0.65
1:B:104:THR:CG2	1:B:118:TYR:OH	2.45	0.65
1:B:16:THR:H	1:B:19:HIS:HD2	1.47	0.61
1:B:71:PHE:CD1	1:B:72:SER:HB2	2.36	0.60
1:D:82:VAL:HG12	1:D:82:VAL:O	2.02	0.59
1:F:9:PRO:HG3	1:F:75:LEU:HD21	1.84	0.58
1:F:7:VAL:HG13	1:F:36:CYS:SG	2.43	0.58
1:A:106:MET:O	1:A:106:MET:HE2	2.03	0.58
1:E:45:GLY:O	1:E:47:PHE:N	2.36	0.58
1:B:71:PHE:CA	1:B:72:SER:HB2	2.33	0.58
1:D:3:HIS:CE1	4:D:306:HOH:O	2.56	0.57
1:E:71:PHE:CG	1:E:72:SER:HB2	2.39	0.57
1:F:49:LEU:HD23	1:F:49:LEU:C	2.26	0.56
1:A:106:MET:HE2	1:A:110:LEU:HD13	1.87	0.56
1:C:119:MET:CE	1:E:115:GLU:HG3	2.36	0.55
1:D:104:THR:OG1	1:D:118:TYR:OH	2.24	0.55
1:D:108:LYS:NZ	1:D:115:GLU:OE2	2.38	0.55
3:A:202:2VJ:H4	1:C:75:LEU:CD2	2.38	0.54
1:B:120:MET:HG3	1:F:104:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:THR:OG1	1:E:29:ARG:NH1	2.41	0.54
1:A:16:THR:H	1:A:19:HIS:HD2	1.55	0.53
1:A:129:SER:HB2	2:A:201:AGS:O2G	2.08	0.53
1:C:16:THR:H	1:C:19:HIS:HD2	1.56	0.53
1:E:104:THR:OG1	1:E:118:TYR:OH	2.24	0.53
3:A:202:2VJ:H23	4:A:301:HOH:O	2.08	0.53
1:A:42:LYS:O	1:A:43:LYS:CB	2.57	0.53
1:A:36[B]:CYS:SG	1:A:37:VAL:N	2.82	0.53
1:C:108:LYS:NZ	4:C:307:HOH:O	2.41	0.52
1:D:76:VAL:HG21	1:D:111:ASN:HB3	1.91	0.52
1:F:16:THR:H	1:F:19:HIS:HD2	1.58	0.51
3:D:202:2VJ:C34	1:E:135:GLU:OE2	2.58	0.51
1:F:135:GLU:CD	3:F:202:2VJ:C36	2.78	0.51
1:E:7:VAL:HG11	1:E:75:LEU:HD11	1.92	0.51
1:A:40:ASN:C	1:A:41:SER:O	2.47	0.51
1:A:106:MET:CE	1:A:110:LEU:HD13	2.40	0.50
1:D:16:THR:H	1:D:19:HIS:HD2	1.60	0.50
1:E:7:VAL:HG12	1:E:9:PRO:HD3	1.94	0.49
2:F:201:AGS:O1A	2:F:201:AGS:O3G	2.29	0.49
1:E:82:VAL:O	1:E:82:VAL:HG12	2.12	0.49
1:A:39:LYS:HD3	1:A:40:ASN:HD22	1.77	0.49
1:E:49:LEU:CD2	1:E:53:MET:SD	3.01	0.49
1:A:44:GLU:HA	1:A:45:GLY:O	2.13	0.49
1:A:9:PRO:HG3	1:A:75:LEU:HD21	1.93	0.49
1:A:8:ILE:HG12	1:A:88:ILE:HB	1.95	0.48
1:E:60:VAL:HG21	1:E:66:VAL:HG11	1.96	0.47
1:B:24:GLU:O	1:B:27:THR:HG22	2.13	0.47
1:B:71:PHE:HA	1:B:72:SER:CB	2.42	0.47
1:D:22:ILE:HD11	2:D:201:AGS:H2	1.96	0.47
1:B:118:TYR:HB2	1:F:118:TYR:HB2	1.97	0.47
1:D:33:ILE:HB	1:D:66:VAL:HG22	1.97	0.47
1:D:75:LEU:CD2	3:D:202:2VJ:H4	2.45	0.46
1:A:44:GLU:HB2	1:A:45:GLY:O	2.15	0.46
1:B:8:ILE:HG12	1:B:88:ILE:HB	1.97	0.45
1:C:49:LEU:HD13	1:C:49:LEU:C	2.36	0.45
1:B:16:THR:H	1:B:19:HIS:CD2	2.32	0.45
1:C:145:GLU:HG2	1:C:146:PHE:CE1	2.50	0.45
1:A:75:LEU:CD2	3:A:203:2VJ:H4	2.47	0.45
1:E:129:SER:OG	1:E:132:ILE:HG22	2.17	0.45
1:C:145:GLU:HG2	1:C:146:PHE:CD1	2.52	0.44
1:E:71:PHE:HA	1:E:72:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ASP:OD2	1:D:29:ARG:NH1	2.49	0.44
1:C:151:VAL:HG12	1:C:155:LEU:HD22	1.99	0.44
1:E:45:GLY:O	1:E:46:THR:C	2.55	0.44
1:A:106:MET:CE	1:A:109:LYS:HB2	2.47	0.44
1:C:38:LEU:HD12	1:C:38:LEU:N	2.22	0.44
1:F:40:ASN:O	1:F:41:SER:C	2.56	0.44
1:A:42:LYS:O	1:A:43:LYS:HB3	2.18	0.43
1:E:71:PHE:HA	1:E:72:SER:CB	2.48	0.43
1:D:75:LEU:HD23	3:D:202:2VJ:H4	1.99	0.43
1:B:58:GLN:HG3	1:B:150:TYR:CZ	2.53	0.43
1:C:60:VAL:CG1	1:C:60:VAL:O	2.65	0.43
1:A:76:VAL:HG21	1:A:110:LEU:HB3	2.01	0.42
1:D:90:GLY:O	2:D:201:AGS:O2'	2.38	0.42
1:B:117:LEU:HD13	1:F:117:LEU:HD13	2.01	0.42
1:A:7:VAL:CG1	1:A:36[A]:CYS:SG	3.05	0.41
1:F:135:GLU:OE1	3:F:202:2VJ:C36	2.68	0.41
1:D:41:SER:HB3	1:D:44:GLU:OE2	2.20	0.41
1:E:98:GLU:OE2	1:F:94:VAL:HB	2.20	0.41
1:B:100:GLU:O	1:B:104:THR:HG23	2.19	0.41
1:B:75:LEU:CD2	3:B:202:2VJ:H4	2.50	0.41
1:D:132:ILE:HD13	1:D:132:ILE:HG21	1.84	0.41
1:C:92:ARG:NH1	2:C:201:AGS:S1G	2.89	0.40
1:E:16:THR:HA	1:E:147:VAL:HG12	2.02	0.40
1:D:47:PHE:HZ	1:D:155:LEU:HD13	1.87	0.40
1:E:15:ILE:HG13	1:E:19:HIS:HB2	2.03	0.40
1:D:160:LYS:HD3	1:D:160:LYS:C	2.42	0.40
1:D:43:LYS:N	1:D:44:GLU:OE1	2.54	0.40
1:E:158:LYS:O	1:E:158:LYS:HD2	2.20	0.40

There are no symmetry-related clashes.

## 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	158/160 (99%)	150 (95%)	5 (3%)	3 (2%)	10	11
1	B	158/160 (99%)	154 (98%)	2 (1%)	2 (1%)	15	19
1	C	158/160 (99%)	148 (94%)	8 (5%)	2 (1%)	15	19
1	D	158/160 (99%)	148 (94%)	8 (5%)	2 (1%)	15	19
1	E	158/160 (99%)	146 (92%)	8 (5%)	4 (2%)	7	6
1	F	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
All	All	948/960 (99%)	899 (95%)	36 (4%)	13 (1%)	14	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	GLU
1	B	72	SER
1	C	39	LYS
1	E	46	THR
1	E	72	SER
1	A	41	SER
1	A	43	LYS
1	A	45	GLY
1	C	140	ARG
1	D	43	LYS
1	D	44	GLU
1	E	62	HIS
1	E	71	PHE

### 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	147/147 (100%)	137 (93%)	10 (7%)	20	28
1	B	147/147 (100%)	139 (95%)	8 (5%)	27	40
1	C	147/147 (100%)	137 (93%)	10 (7%)	20	28
1	D	147/147 (100%)	136 (92%)	11 (8%)	17	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	147/147 (100%)	132 (90%)	15 (10%)	9	12
1	F	147/147 (100%)	141 (96%)	6 (4%)	37	54
All	All	882/882 (100%)	822 (93%)	60 (7%)	20	28

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	39	LYS
1	A	42	LYS
1	A	55	LEU
1	A	61	LYS
1	A	80	GLU
1	A	103	LEU
1	A	110	LEU
1	A	140	ARG
1	A	155	LEU
1	B	20	LEU
1	B	39	LYS
1	B	44	GLU
1	B	57	GLU
1	B	82	VAL
1	B	108	LYS
1	B	155	LEU
1	B	158	LYS
1	C	20	LEU
1	C	26	SER
1	C	38	LEU
1	C	43	LYS
1	C	60	VAL
1	C	85	LYS
1	C	131	SER
1	C	140	ARG
1	C	155	LEU
1	C	160	LYS
1	D	44	GLU
1	D	67	LYS
1	D	72	SER
1	D	76	VAL
1	D	111	ASN
1	D	135	GLU

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Mol	Chain	Res	Type
1	D	145	GLU
1	D	155	LEU
1	D	157	LYS
1	D	158	LYS
1	D	160	LYS
1	E	28	ASP
1	E	39	LYS
1	E	41	SER
1	E	42	LYS
1	E	60	VAL
1	E	62	HIS
1	E	76	VAL
1	E	85	LYS
1	E	95	SER
1	E	98	GLU
1	E	115	GLU
1	E	123	THR
1	E	130	SER
1	E	149	PRO
1	E	151	VAL
1	F	28	ASP
1	F	41	SER
1	F	53	MET
1	F	72	SER
1	F	145	GLU
1	F	155	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	40	ASN
1	B	19	HIS
1	B	107	ASN
1	C	19	HIS
1	C	40	ASN
1	C	124	ASN
1	D	19	HIS
1	D	81	GLN
1	D	111	ASN
1	D	124	ASN
1	E	19	HIS

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Mol	Chain	Res	Type
1	E	62	HIS
1	E	70	GLN
1	E	81	GLN
1	F	19	HIS
1	F	124	ASN

### 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](#)

12 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	AGS	A	201	-	24,33,33	1.31	4 (16%)	28,52,52	3.13	7 (25%)
3	2VJ	A	202	-	34,38,38	0.88	2 (5%)	37,53,53	2.01	11 (29%)
3	2VJ	A	203	-	34,38,38	1.07	3 (8%)	37,53,53	2.14	12 (32%)
2	AGS	B	201	-	24,33,33	1.51	6 (25%)	28,52,52	2.60	8 (28%)
3	2VJ	B	202	-	34,38,38	1.14	2 (5%)	37,53,53	2.51	16 (43%)
2	AGS	C	201	-	24,33,33	1.65	6 (25%)	28,52,52	2.66	6 (21%)
2	AGS	D	201	-	24,33,33	1.35	4 (16%)	28,52,52	3.06	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	2VJ	D	202	-	34,38,38	1.08	4 (11%)	37,53,53	2.29	10 (27%)
2	AGS	E	201	-	24,33,33	1.60	5 (20%)	28,52,52	2.79	8 (28%)
2	AGS	F	201	-	24,33,33	1.62	4 (16%)	28,52,52	3.24	13 (46%)
3	2VJ	F	202	-	34,38,38	1.16	4 (11%)	37,53,53	1.87	10 (27%)
3	2VJ	F	203	-	34,38,38	0.79	0	37,53,53	1.80	10 (27%)

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	AGS	A	201	-	-	0/15/38/38	0/3/3/3
3	2VJ	A	202	-	-	0/15/34/34	0/4/4/4
3	2VJ	A	203	-	-	0/15/34/34	0/4/4/4
2	AGS	B	201	-	-	0/15/38/38	0/3/3/3
3	2VJ	B	202	-	-	0/15/34/34	0/4/4/4
2	AGS	C	201	-	-	0/15/38/38	0/3/3/3
2	AGS	D	201	-	-	0/15/38/38	0/3/3/3
3	2VJ	D	202	-	-	0/15/34/34	0/4/4/4
2	AGS	E	201	-	-	0/15/38/38	0/3/3/3
2	AGS	F	201	-	-	0/15/38/38	0/3/3/3
3	2VJ	F	202	-	-	0/15/34/34	0/4/4/4
3	2VJ	F	203	-	-	0/15/34/34	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	202	2VJ	C5-S29	-3.84	1.72	1.77
2	B	201	AGS	C4-N3	-3.50	1.30	1.35
2	C	201	AGS	C4-N3	-3.45	1.30	1.35
2	C	201	AGS	PG-S1G	-2.87	1.85	1.90
3	F	202	2VJ	C5-N6	-2.79	1.31	1.34
2	E	201	AGS	C4-N3	-2.72	1.31	1.35
3	D	202	2VJ	C3-N8	-2.61	1.30	1.34
3	F	202	2VJ	C7-N6	-2.54	1.29	1.34
2	A	201	AGS	C8-N7	-2.41	1.30	1.34
3	B	202	2VJ	C5-S29	-2.38	1.74	1.77
2	F	201	AGS	C8-N7	-2.27	1.30	1.34
3	F	202	2VJ	C15-C9	-2.22	1.52	1.55
2	E	201	AGS	C8-N7	-2.15	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	AGS	C8-N7	-2.14	1.30	1.34
2	D	201	AGS	C8-N7	-2.13	1.30	1.34
3	A	203	2VJ	C7-N6	-2.13	1.30	1.34
3	A	202	2VJ	C7-N6	-2.06	1.30	1.34
3	D	202	2VJ	C7-N8	-2.04	1.30	1.34
2	D	201	AGS	PG-S1G	-2.03	1.86	1.90
3	D	202	2VJ	C7-N6	-2.00	1.30	1.34
3	B	202	2VJ	C7-N6	-2.00	1.30	1.34
3	A	203	2VJ	C23-C22	2.00	1.42	1.38
2	C	201	AGS	O4'-C1'	2.02	1.43	1.41
2	B	201	AGS	PB-O2B	2.09	1.63	1.54
2	A	201	AGS	PG-O3G	2.11	1.62	1.55
2	A	201	AGS	PG-O2G	2.11	1.62	1.55
2	F	201	AGS	PB-O2B	2.14	1.64	1.54
2	B	201	AGS	O4'-C1'	2.18	1.44	1.41
3	A	202	2VJ	C34-C33	2.25	1.41	1.37
2	B	201	AGS	PG-O3G	2.40	1.63	1.55
2	B	201	AGS	C2-N3	2.43	1.36	1.32
3	D	202	2VJ	C25-CL7	2.52	1.79	1.73
2	D	201	AGS	PA-O1A	2.83	1.61	1.51
2	D	201	AGS	O4'-C1'	2.84	1.44	1.41
2	E	201	AGS	PB-O1B	2.84	1.61	1.51
2	E	201	AGS	O4'-C1'	2.92	1.44	1.41
2	C	201	AGS	PB-O1B	3.10	1.62	1.51
2	C	201	AGS	PG-O3G	3.23	1.66	1.55
2	F	201	AGS	PG-O3G	3.23	1.66	1.55
2	A	201	AGS	PB-O1B	3.25	1.63	1.51
2	B	201	AGS	PG-O2G	3.39	1.67	1.55
2	E	201	AGS	PG-O2G	3.51	1.67	1.55
3	A	203	2VJ	C30-S29	3.71	1.81	1.76
2	F	201	AGS	O4'-C1'	4.80	1.47	1.41

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	AGS	N3-C2-N1	-9.93	121.29	128.89
2	D	201	AGS	PA-O3A-PB	-9.21	106.86	132.73
2	A	201	AGS	PB-O3B-PG	-8.46	104.30	132.67
2	D	201	AGS	N3-C2-N1	-8.37	122.48	128.89
2	F	201	AGS	PB-O3B-PG	-8.10	105.51	132.67
3	B	202	2VJ	C4-C5-S29	-8.02	113.20	124.19
2	E	201	AGS	PB-O3B-PG	-7.91	106.13	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	AGS	PB-O3B-PG	-7.71	106.82	132.67
2	A	201	AGS	PA-O3A-PB	-7.60	111.39	132.73
2	C	201	AGS	PB-O3B-PG	-7.57	107.29	132.67
2	C	201	AGS	PA-O3A-PB	-7.18	112.58	132.73
2	B	201	AGS	PB-O3B-PG	-7.14	108.73	132.67
3	D	202	2VJ	C4-C5-S29	-7.07	114.50	124.19
2	C	201	AGS	N3-C2-N1	-6.88	123.63	128.89
2	B	201	AGS	PA-O3A-PB	-6.81	113.60	132.73
2	E	201	AGS	PA-O3A-PB	-6.72	113.86	132.73
2	E	201	AGS	N3-C2-N1	-6.67	123.79	128.89
3	A	203	2VJ	C4-C5-N6	-6.64	118.61	123.66
2	F	201	AGS	N3-C2-N1	-6.48	123.93	128.89
3	A	202	2VJ	C4-C5-N6	-6.17	118.98	123.66
3	B	202	2VJ	C20-C21-C26	-5.29	111.24	120.62
2	F	201	AGS	C2'-C1'-N9	-5.27	106.23	114.29
3	F	202	2VJ	C4-C5-S29	-5.16	117.12	124.19
3	F	203	2VJ	C25-C26-C21	-5.13	117.05	120.36
2	B	201	AGS	N3-C2-N1	-4.62	125.36	128.89
2	F	201	AGS	C4'-O4'-C1'	-4.20	105.10	109.72
2	B	201	AGS	C4-C5-N7	-4.18	105.63	109.48
3	A	203	2VJ	C20-C21-C26	-4.15	113.26	120.62
2	D	201	AGS	C4'-O4'-C1'	-4.03	105.30	109.72
3	F	203	2VJ	C4-C5-N6	-3.92	120.69	123.66
3	A	202	2VJ	C4-C3-N8	-3.82	118.65	122.96
3	F	202	2VJ	C25-C26-C21	-3.79	117.92	120.36
3	D	202	2VJ	C4-C3-N8	-3.75	118.73	122.96
3	A	203	2VJ	C25-C24-CL8	-3.72	111.58	120.87
3	D	202	2VJ	C9-C15-C17	-3.72	105.62	111.51
3	B	202	2VJ	N6-C7-N8	-3.60	120.72	126.08
2	E	201	AGS	C4'-O4'-C1'	-3.59	105.78	109.72
2	B	201	AGS	C4'-O4'-C1'	-3.57	105.80	109.72
2	E	201	AGS	C4-C5-N7	-3.53	106.23	109.48
3	A	202	2VJ	C11-C9-C7	-3.46	103.78	112.01
3	D	202	2VJ	C12-C11-C9	-3.46	106.97	111.62
3	F	202	2VJ	C4-C3-N8	-3.44	119.08	122.96
2	A	201	AGS	C4'-O4'-C1'	-3.37	106.02	109.72
2	F	201	AGS	C5'-C4'-C3'	-3.37	101.85	115.21
3	A	202	2VJ	C4-C5-S29	-3.34	119.61	124.19
3	B	202	2VJ	C9-C15-C17	-3.28	106.31	111.51
2	C	201	AGS	C4'-O4'-C1'	-3.24	106.16	109.72
2	F	201	AGS	PA-O3A-PB	-3.23	123.65	132.73
3	A	203	2VJ	N6-C7-N8	-3.18	121.35	126.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	202	2VJ	C4-C5-N6	-3.18	121.24	123.66
2	B	201	AGS	C2'-C1'-N9	-3.12	109.52	114.29
3	F	203	2VJ	C4-C5-S29	-3.03	120.03	124.19
3	A	202	2VJ	N6-C7-N8	-2.99	121.63	126.08
3	A	203	2VJ	C13-C12-C11	-2.96	105.23	111.44
3	B	202	2VJ	C2-C3-C4	-2.85	116.13	122.70
3	D	202	2VJ	C9-C7-N8	-2.80	114.13	116.97
3	F	202	2VJ	C11-C9-C7	-2.73	105.52	112.01
3	B	202	2VJ	C12-C13-C14	-2.68	105.82	111.44
3	A	202	2VJ	C25-C26-C21	-2.66	118.64	120.36
3	F	203	2VJ	C11-C9-C7	-2.63	105.76	112.01
3	F	203	2VJ	C4-C3-N8	-2.62	120.00	122.96
3	B	202	2VJ	C25-C24-CL8	-2.59	114.39	120.87
2	B	201	AGS	O2A-PA-O3A	-2.58	93.39	105.09
2	D	201	AGS	C4-C5-N7	-2.57	107.11	109.48
2	D	201	AGS	C2'-C1'-N9	-2.56	110.38	114.29
3	F	203	2VJ	C22-C23-C24	-2.52	116.20	119.95
3	F	203	2VJ	N6-C7-N8	-2.46	122.42	126.08
2	F	201	AGS	O2A-PA-O5'	-2.45	96.09	108.46
3	D	202	2VJ	C20-C21-C22	-2.43	115.50	120.90
2	F	201	AGS	C2'-C3'-C4'	-2.42	97.64	102.61
3	F	202	2VJ	C14-C15-C17	-2.32	105.93	111.31
3	A	202	2VJ	C22-C23-C24	-2.27	116.56	119.95
3	B	202	2VJ	C23-C22-C21	-2.21	118.01	121.04
2	E	201	AGS	C1'-N9-C4	-2.21	123.61	126.94
3	B	202	2VJ	C13-C12-C11	-2.20	106.82	111.44
3	D	202	2VJ	O18-C17-C15	-2.19	119.04	121.56
2	E	201	AGS	C2'-C1'-N9	-2.17	110.98	114.29
3	A	203	2VJ	C4-C3-N8	-2.16	120.52	122.96
3	F	202	2VJ	C14-C15-C9	-2.16	107.20	109.63
3	F	202	2VJ	C2-C3-C4	-2.15	117.74	122.70
3	B	202	2VJ	C11-C9-C7	-2.15	106.91	112.01
3	F	203	2VJ	C12-C11-C9	-2.15	108.74	111.62
2	C	201	AGS	C4-C5-N7	-2.11	107.53	109.48
3	B	202	2VJ	C4-C5-N6	-2.11	122.06	123.66
2	A	201	AGS	C2'-C3'-C4'	-2.08	98.33	102.61
2	F	201	AGS	C4-C5-N7	-2.08	107.57	109.48
3	F	202	2VJ	N6-C7-N8	-2.08	122.99	126.08
3	B	202	2VJ	C1-C2-C3	-2.07	105.79	113.54
3	A	203	2VJ	C12-C13-C14	-2.05	107.15	111.44
3	D	202	2VJ	N6-C7-N8	-2.01	123.10	126.08
3	A	203	2VJ	C26-C25-CL7	2.00	121.59	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	2VJ	C23-C24-C25	2.01	123.96	120.00
3	A	203	2VJ	O18-C17-C15	2.03	123.89	121.56
2	A	201	AGS	O4'-C4'-C3'	2.18	109.54	105.15
3	F	203	2VJ	C26-C25-C24	2.20	123.54	120.25
2	C	201	AGS	O3G-PG-O3B	2.20	115.06	105.09
2	A	201	AGS	O2G-PG-O3B	2.21	115.12	105.09
3	A	202	2VJ	C22-C21-C26	2.23	121.84	118.55
2	B	201	AGS	O2B-PB-O3A	2.30	115.52	105.09
3	F	203	2VJ	C9-C7-N8	2.33	119.33	116.97
2	D	201	AGS	O3A-PA-O5'	2.49	109.55	102.94
2	E	201	AGS	O2G-PG-O3B	2.51	116.49	105.09
3	A	203	2VJ	C9-C7-N8	2.62	119.62	116.97
3	A	203	2VJ	C20-C21-C22	2.76	127.03	120.90
3	B	202	2VJ	C2-C3-N8	2.82	122.62	116.09
3	A	202	2VJ	C2-C3-N8	2.83	122.65	116.09
2	F	201	AGS	O5'-C5'-C4'	2.90	119.80	109.12
3	A	202	2VJ	C9-C7-N8	2.91	119.92	116.97
3	F	202	2VJ	C2-C3-N8	3.06	123.18	116.09
3	B	202	2VJ	C20-C21-C22	3.12	127.82	120.90
2	F	201	AGS	O2A-PA-O3A	3.51	121.03	105.09
3	B	202	2VJ	C9-C7-N6	3.71	120.73	116.97
3	A	203	2VJ	C23-C24-CL8	3.74	126.13	118.39
3	B	202	2VJ	C23-C24-CL8	3.88	126.41	118.39
3	F	202	2VJ	C9-C7-N8	4.36	121.39	116.97
2	F	201	AGS	O4'-C1'-N9	4.54	117.60	108.10
3	D	202	2VJ	C9-C7-N6	5.71	122.76	116.97
2	F	201	AGS	O3A-PA-O5'	6.79	120.95	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	AGS	4	0
3	A	202	2VJ	3	0
3	A	203	2VJ	3	0
3	B	202	2VJ	1	0
2	C	201	AGS	1	0
2	D	201	AGS	3	0
3	D	202	2VJ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	201	AGS	1	0
3	F	202	2VJ	2	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 ⓘ

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	159/160 (99%)	0.26	4 (2%) 61 64	21, 35, 50, 50	0
1	B	160/160 (100%)	0.43	14 (8%) 12 14	20, 33, 50, 50	0
1	C	160/160 (100%)	0.43	11 (6%) 20 22	22, 38, 50, 50	0
1	D	159/160 (99%)	0.40	6 (3%) 44 49	20, 38, 50, 50	0
1	E	160/160 (100%)	0.84	19 (11%) 6 7	27, 46, 50, 50	0
1	F	160/160 (100%)	0.52	16 (10%) 9 10	22, 39, 50, 50	0
All	All	958/960 (99%)	0.48	70 (7%) 18 20	20, 38, 50, 50	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	ASN	6.7
1	E	1	MET	6.6
1	E	160	LYS	5.8
1	B	1	MET	5.6
1	C	160	LYS	4.9
1	E	40	ASN	4.8
1	C	39	LYS	4.7
1	A	44	GLU	4.3
1	F	40	ASN	4.3
1	D	42	LYS	4.2
1	B	2	GLU	4.1
1	E	157	LYS	4.0
1	B	44	GLU	3.8
1	B	160	LYS	3.8
1	E	42	LYS	3.8
1	A	43	LYS	3.5
1	F	38	LEU	3.5
1	E	43	LYS	3.5
1	F	39	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	160	LYS	3.4
1	E	47	PHE	3.4
1	E	2	GLU	3.3
1	C	140	ARG	3.3
1	D	43	LYS	3.1
1	C	44	GLU	3.1
1	F	157	LYS	3.1
1	C	41	SER	3.1
1	E	41	SER	3.0
1	E	151	VAL	3.0
1	A	42	LYS	3.0
1	F	155	LEU	2.9
1	E	44	GLU	2.8
1	C	72	SER	2.8
1	F	44	GLU	2.8
1	C	43	LYS	2.8
1	F	42	LYS	2.8
1	D	40	ASN	2.8
1	E	159	PHE	2.7
1	E	39	LYS	2.7
1	B	150	TYR	2.7
1	E	48	SER	2.6
1	F	72	SER	2.6
1	E	3	HIS	2.5
1	B	49	LEU	2.5
1	B	42	LYS	2.5
1	A	45	GLY	2.5
1	E	150	TYR	2.4
1	C	42	LYS	2.4
1	D	160	LYS	2.4
1	E	155	LEU	2.4
1	B	40	ASN	2.4
1	F	150	TYR	2.3
1	F	41	SER	2.3
1	B	45	GLY	2.2
1	B	41	SER	2.2
1	D	2	GLU	2.2
1	D	150	TYR	2.2
1	B	94	VAL	2.2
1	F	145	GLU	2.2
1	C	71	PHE	2.2
1	E	45	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	43	LYS	2.2
1	F	46	THR	2.2
1	B	72	SER	2.1
1	E	153	LYS	2.1
1	F	153	LYS	2.1
1	C	95	SER	2.0
1	F	73	GLY	2.0
1	B	97	PHE	2.0
1	F	94	VAL	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, 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(Å <sup>2</sup> )	Q<0.9
3	2VJ	A	203	35/35	0.84	0.21	1.82	25,35,50,50	0
3	2VJ	F	202	35/35	0.81	0.22	1.75	35,44,50,50	0
2	AGS	F	201	31/31	0.88	0.17	1.22	34,42,50,50	0
3	2VJ	D	202	35/35	0.82	0.20	1.17	25,39,50,50	0
2	AGS	D	201	31/31	0.88	0.17	1.10	24,33,50,50	0
2	AGS	E	201	31/31	0.88	0.17	0.55	28,42,50,50	0
3	2VJ	A	202	35/35	0.86	0.19	0.41	30,40,50,50	0
2	AGS	A	201	31/31	0.88	0.15	0.37	26,37,50,50	0
3	2VJ	F	203	35/35	0.83	0.18	0.35	32,39,50,50	0
2	AGS	C	201	31/31	0.91	0.15	0.13	32,40,50,50	0
2	AGS	B	201	31/31	0.93	0.14	0.07	21,29,50,50	0
3	2VJ	B	202	35/35	0.88	0.16	-0.11	24,31,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.