



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:18 pm BST

PDB ID : 5VWQ  
Title : E.coli Aspartate aminotransferase-(1R,3S,4S)-3-amino-4-fluorocyclopentane-1-carboxylic acid (FCP)  
Authors : Mascarenhas, R.; Lehrer, H.; Liu, D.; Ringe, D.  
Deposited on : 2017-05-22  
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

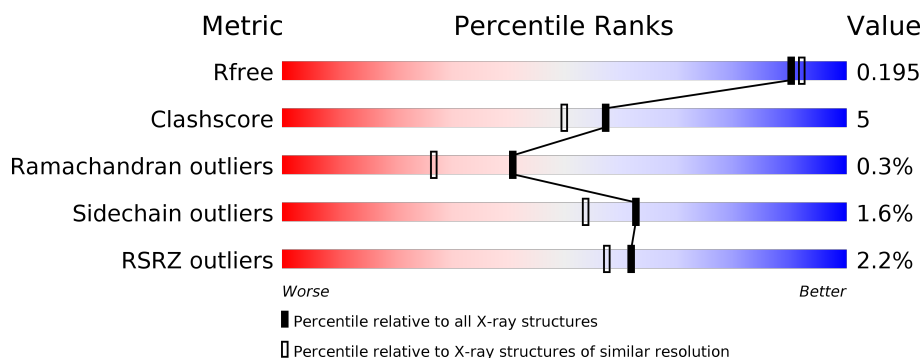
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>1%</span> <span>88%</span> <span>11%</span> </div> </div>
1	D	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>3%</span> <span>87%</span> <span>11%</span> </div> </div>
1	G	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 96%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>90%</span> <span>9%</span> </div> </div>
1	J	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>3%</span> <span>88%</span> <span>11%</span> </div> </div>

## 2 Entry composition [i](#)

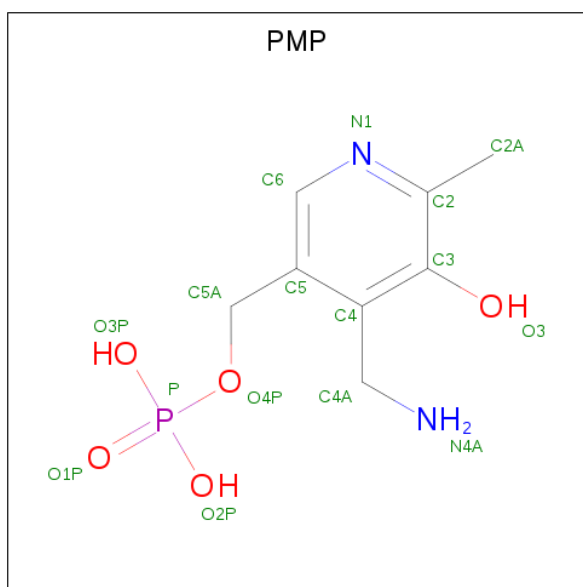
There are 3 unique types of molecules in this entry. The entry contains 15182 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aspartate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	54	0
			3422	2184	587	634	17			
1	D	396	Total	C	N	O	S	0	56	0
			3437	2197	588	635	17			
1	G	396	Total	C	N	O	S	0	56	0
			3426	2192	586	631	17			
1	J	396	Total	C	N	O	S	0	52	0
			3399	2172	580	631	16			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	J	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

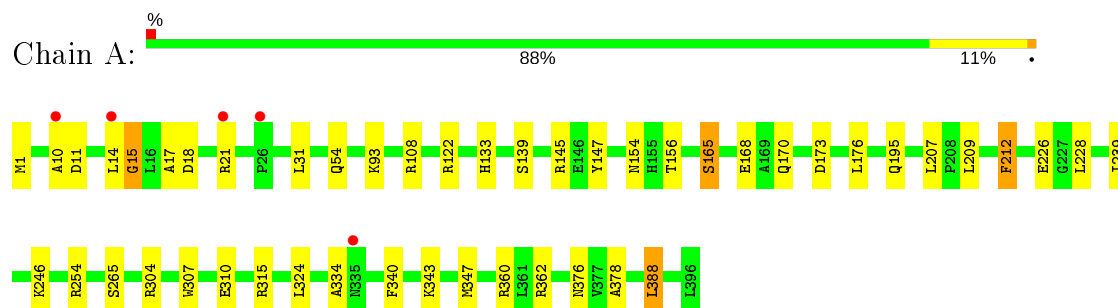
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	364	Total	O	0	0
			364	364		
3	D	370	Total	O	0	0
			370	370		
3	G	346	Total	O	0	0
			346	346		
3	J	354	Total	O	0	0
			354	354		

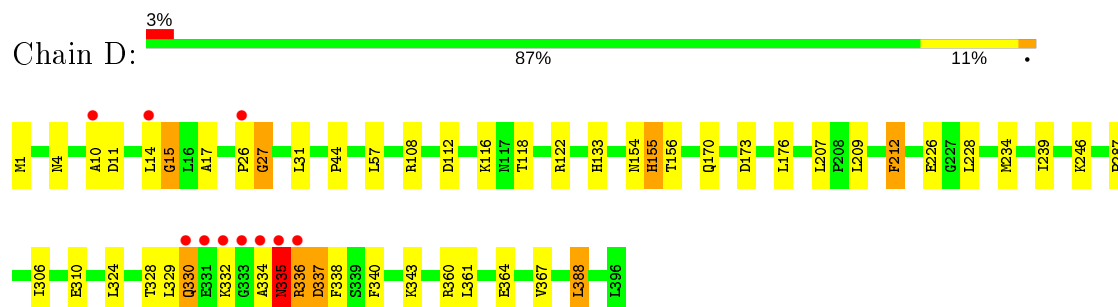
### 3 Residue-property plots [i](#)

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.

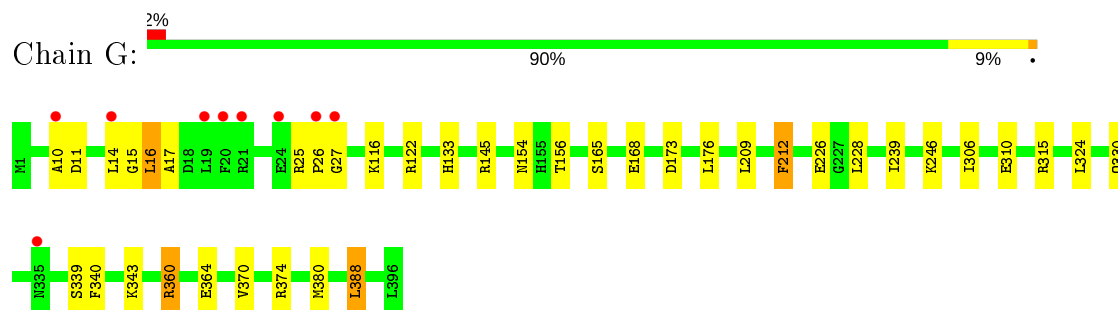
- Molecule 1: Aspartate aminotransferase



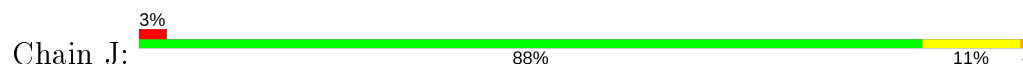
- Molecule 1: Aspartate aminotransferase

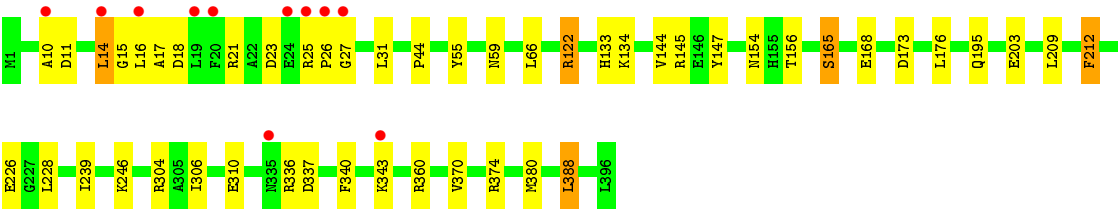


- Molecule 1: Aspartate aminotransferase



- Molecule 1: Aspartate aminotransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.90Å 84.90Å 88.03Å 118.83° 90.10° 89.59°	Depositor
Resolution (Å)	29.39 – 1.80 29.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.39-1.80) 94.6 (29.39-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.162 , 0.192 0.168 , 0.195	Depositor DCC
$R_{free}$ test set	9000 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-l,k+l 0.008 for h,k+l,-k 0.007 for h,-k-l,k 0.007 for h,l,-k-l 0.419 for h,-k,-l 0.419 for -h,k,-k-l 0.009 for -h,-k-l,l 0.008 for -h,-l,-k 0.009 for -h,l,k 0.448 for -h,-k,k+l 0.007 for -h,k+l,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: PMP

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	0.76	0/3627	0.79	14/4896 (0.3%)
1	D	0.78	0/3646	0.79	3/4922 (0.1%)
1	G	0.76	0/3641	0.76	6/4916 (0.1%)
1	J	0.77	0/3596	0.75	2/4857 (0.0%)
All	All	0.77	0/14510	0.77	25/19591 (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	D	0	3
1	G	0	1
1	J	0	1
All	All	0	5

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLY	N-CA-C	-8.52	91.81	113.10
1	D	15	GLY	N-CA-C	-7.72	93.79	113.10
1	A	304[A]	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	304[C]	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	304[B]	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	315[A]	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	315[B]	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	315[C]	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	G	315[A]	ARG	NE-CZ-NH2	-6.50	117.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	315[B]	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	G	315[C]	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	315[A]	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	315[B]	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	315[C]	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	G	315[A]	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	G	315[B]	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	G	315[C]	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	D	27	GLY	N-CA-C	-5.99	98.12	113.10
1	J	16	LEU	CA-CB-CG	5.21	127.28	115.30
1	D	335	ASN	N-CA-CB	-5.13	101.36	110.60
1	A	304[A]	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	304[C]	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	304[B]	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	334	ALA	N-CA-C	-5.08	97.28	111.00
1	J	66	LEU	CB-CG-CD1	-5.05	102.42	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	329	LEU	Peptide
1	D	330	GLN	Peptide
1	G	25	ARG	Peptide
1	J	14	LEU	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	3422	0	3524	43	0
1	D	3437	0	3541	58	0
1	G	3426	0	3536	22	0
1	J	3399	0	3486	30	0
2	A	16	0	10	2	0
2	D	16	0	10	2	0
2	G	16	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	16	0	10	2	0
3	A	364	0	0	4	0
3	D	370	0	0	13	1
3	G	346	0	0	3	2
3	J	354	0	0	6	1
All	All	15182	0	14127	137	2

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 5.

All (137) 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:D:335:ASN:O	3:D:501:HOH:O	1.74	1.05
1:D:335:ASN:ND2	3:D:503:HOH:O	2.03	0.92
1:D:330:GLN:OE1	3:D:501:HOH:O	1.90	0.90
1:D:330:GLN:HB2	1:D:334:ALA:HB3	1.53	0.89
1:D:332:LYS:O	3:D:502:HOH:O	1.90	0.89
1:A:108[B]:ARG:HH21	1:D:108[B]:ARG:HH21	1.22	0.87
1:J:336:ARG:NH2	3:J:501:HOH:O	2.13	0.82
1:J:23:ASP:OD1	1:J:25:ARG:HG3	1.82	0.79
1:D:335:ASN:OD1	1:D:336:ARG:N	2.15	0.78
1:J:18:ASP:OD1	1:J:21:ARG:NH2	2.15	0.78
1:A:1[D]:MET:SD	1:D:207:LEU:HD22	2.25	0.77
1:A:145[A]:ARG:NH1	1:A:168[A]:GLU:OE1	2.18	0.73
1:D:337:ASP:N	3:D:501:HOH:O	2.21	0.72
1:A:207:LEU:HD22	1:D:1[D]:MET:SD	2.31	0.71
1:D:330:GLN:HE22	1:D:337:ASP:HA	1.56	0.71
1:A:108[B]:ARG:HH21	1:D:108[B]:ARG:NH2	1.90	0.69
1:D:246:LYS:NZ	2:D:401:PMP:HNA2	1.91	0.69
1:G:246:LYS:NZ	2:G:401:PMP:HNA2	1.91	0.69
1:A:108[B]:ARG:NH2	1:D:108[B]:ARG:HH21	1.90	0.68
1:A:212[B]:PHE:HE2	1:A:228:LEU:HB2	1.62	0.65
1:A:209[B]:LEU:HD22	1:A:239:ILE:HB	1.79	0.65
1:D:336:ARG:NH1	3:D:505:HOH:O	2.26	0.64
1:D:209[B]:LEU:HD22	1:D:239:ILE:HB	1.80	0.63
1:J:246:LYS:NZ	2:J:401:PMP:HNA2	1.96	0.62
1:D:212[B]:PHE:HE2	1:D:228:LEU:HB2	1.64	0.62
1:J:212[B]:PHE:HE2	1:J:228:LEU:HB2	1.63	0.62
1:J:212[B]:PHE:CE2	1:J:228:LEU:HB2	2.36	0.60
1:D:330:GLN:HE22	1:D:338:PHE:H	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:GLN:NE2	3:G:510:HOH:O	2.34	0.60
1:D:330:GLN:NE2	1:D:338:PHE:H	1.99	0.60
1:J:14:LEU:O	1:J:17:ALA:HB3	2.02	0.59
1:A:18:ASP:HA	1:A:21:ARG:NH1	2.17	0.59
1:D:212[B]:PHE:CE2	1:D:228:LEU:HB2	2.38	0.59
1:G:212[B]:PHE:HE2	1:G:228:LEU:HB2	1.67	0.59
1:G:15:GLY:HA2	1:G:17:ALA:N	2.18	0.58
1:J:226[B]:GLU:HG2	3:J:647:HOH:O	2.03	0.58
1:G:306:ILE:O	1:G:310[B]:GLU:HG3	2.02	0.58
1:G:145[A]:ARG:NH1	1:G:168[A]:GLU:OE1	2.25	0.58
1:D:336:ARG:O	1:D:337:ASP:HB3	2.04	0.58
1:D:234[A]:MET:SD	3:D:832:HOH:O	2.57	0.57
1:A:226[B]:GLU:HG2	3:A:686:HOH:O	2.04	0.57
1:A:18:ASP:OD1	1:A:21:ARG:NH1	2.31	0.57
1:A:122[A]:ARG:NH1	1:A:173:ASP:OD1	2.37	0.56
1:J:14:LEU:N	1:J:15:GLY:HA3	2.19	0.56
1:A:376[B]:ASN:ND2	1:A:378:ALA:H	2.04	0.56
1:D:328:THR:O	1:D:332:LYS:HG2	2.06	0.56
1:G:209[B]:LEU:HD22	1:G:239:ILE:HB	1.86	0.56
1:D:332:LYS:O	1:D:332:LYS:HG3	2.05	0.55
1:J:209[B]:LEU:HD22	1:J:239:ILE:HB	1.89	0.55
1:A:108[B]:ARG:HH21	1:D:108[B]:ARG:HE	1.55	0.55
1:A:246:LYS:NZ	2:A:401:PMP:HNA2	2.04	0.55
1:D:246:LYS:HZ3	2:D:401:PMP:HNA2	1.52	0.54
1:J:145[A]:ARG:NH1	1:J:168[A]:GLU:OE1	2.30	0.54
1:D:364[A]:GLU:HG2	3:D:590:HOH:O	2.08	0.53
1:D:116[A]:LYS:HD2	3:D:766:HOH:O	2.09	0.52
1:D:306:ILE:O	1:D:310[B]:GLU:HG3	2.10	0.52
1:J:55:TYR:CE1	1:J:59[A]:ASN:ND2	2.76	0.52
1:G:246:LYS:HZ2	2:G:401:PMP:HNA2	1.57	0.52
1:A:133:HIS:CE1	1:A:176[B]:LEU:HD21	2.45	0.52
1:D:14:LEU:N	1:D:15:GLY:HA3	2.25	0.52
1:J:10:ALA:O	1:J:11:ASP:HB3	2.09	0.52
1:D:340:PHE:O	1:D:343[A]:LYS:HG2	2.09	0.51
1:A:14:LEU:O	1:A:17:ALA:HB3	2.10	0.51
1:A:108[B]:ARG:HE	1:D:108[B]:ARG:HH21	1.58	0.51
1:A:108[B]:ARG:HE	1:D:108[B]:ARG:NH2	2.08	0.51
1:A:362[B]:ARG:NH2	3:A:512:HOH:O	2.43	0.51
1:D:330:GLN:HE22	1:D:338:PHE:N	2.09	0.51
1:D:133:HIS:CE1	1:D:176[B]:LEU:HD21	2.46	0.51
1:J:154:ASN:O	1:J:156[B]:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASN:O	1:A:156[B]:THR:HG23	2.12	0.50
1:G:15:GLY:HA2	1:G:16:LEU:C	2.32	0.50
1:J:380:MET:HG2	1:J:388[B]:LEU:HD11	1.93	0.49
1:G:154:ASN:O	1:G:156[B]:THR:HG23	2.11	0.49
1:J:306:ILE:O	1:J:310[B]:GLU:HG3	2.14	0.48
1:D:154:ASN:O	1:D:156[B]:THR:HG23	2.14	0.48
1:A:108[B]:ARG:NH2	1:D:112:ASP:OD2	2.45	0.48
1:D:155[A]:HIS:ND1	1:D:155[A]:HIS:N	2.61	0.47
1:A:108[B]:ARG:NH2	1:D:108[B]:ARG:HE	2.12	0.47
1:G:340:PHE:O	1:G:343[A]:LYS:HG2	2.14	0.47
1:A:122[A]:ARG:NH1	1:A:170:GLN:OE1	2.48	0.47
1:G:122[A]:ARG:NH1	1:G:173:ASP:OD1	2.47	0.47
1:G:14:LEU:O	1:G:17:ALA:HB3	2.15	0.47
1:G:360[A]:ARG:NH1	1:G:364[A]:GLU:OE1	2.42	0.47
1:G:26:PRO:HA	1:G:27:GLY:HA2	1.69	0.47
1:D:122[A]:ARG:NH1	1:D:173:ASP:OD1	2.47	0.47
1:D:4:ASN:HB2	3:D:800:HOH:O	2.14	0.46
1:G:226[B]:GLU:HG2	3:G:566:HOH:O	2.15	0.46
1:A:340:PHE:O	1:A:343[A]:LYS:HG2	2.15	0.46
1:G:10:ALA:O	1:G:11:ASP:HB3	2.16	0.46
1:J:340:PHE:O	1:J:343[A]:LYS:HG2	2.16	0.46
1:J:246:LYS:HZ3	2:J:401:PMP:HNA2	1.63	0.45
1:G:370[B]:VAL:CG2	1:G:374:ARG:HB3	2.46	0.45
1:J:122[A]:ARG:NH1	1:J:173:ASP:OD1	2.50	0.45
1:J:370[B]:VAL:CG2	1:J:374:ARG:HB3	2.47	0.45
1:A:14:LEU:N	1:A:15:GLY:HA3	2.31	0.45
1:J:133:HIS:CE1	1:J:176[B]:LEU:HD21	2.52	0.45
1:D:10:ALA:O	1:D:11:ASP:HB3	2.17	0.44
1:A:54[B]:GLN:NE2	1:D:57:LEU:HD21	2.32	0.44
1:G:133:HIS:CE1	1:G:176[B]:LEU:HD21	2.52	0.44
1:J:134[B]:LYS:HD2	3:J:761:HOH:O	2.16	0.44
1:D:26:PRO:HA	1:D:27:GLY:HA2	1.75	0.44
1:G:380:MET:HG2	1:G:388[B]:LEU:HD11	1.98	0.44
1:A:195:GLN:HG2	3:A:809:HOH:O	2.16	0.44
1:A:108[B]:ARG:HH21	1:D:108[B]:ARG:NE	2.14	0.44
1:A:212[B]:PHE:CE2	1:A:228:LEU:HB2	2.47	0.44
1:A:246:LYS:HZ3	2:A:401:PMP:HNA2	1.65	0.44
1:A:31:LEU:HD11	1:A:388[A]:LEU:HD21	2.01	0.43
1:D:116[A]:LYS:HD3	1:D:116[A]:LYS:HA	1.66	0.43
1:D:14:LEU:O	1:D:17:ALA:HB3	2.18	0.43
1:J:147:TYR:HB2	1:J:165[B]:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TRP:HA	1:A:310[B]:GLU:OE1	2.19	0.43
1:D:155[A]:HIS:CD2	1:D:340:PHE:CE2	3.06	0.42
1:J:31:LEU:HD11	1:J:388[A]:LEU:HD21	2.01	0.42
1:A:10:ALA:O	1:A:11:ASP:HB3	2.20	0.42
1:A:108[B]:ARG:NE	1:D:108[B]:ARG:HH21	2.17	0.42
1:A:147:TYR:HB2	1:A:165[B]:SER:OG	2.19	0.42
1:A:108[B]:ARG:HH21	1:D:108[B]:ARG:CZ	2.33	0.42
1:A:139[B]:SER:OG	3:A:501:HOH:O	2.21	0.42
1:A:347[B]:MET:HB3	1:A:376[B]:ASN:ND2	2.35	0.42
1:J:304[A]:ARG:NH2	3:J:510:HOH:O	2.40	0.42
1:A:93:LYS:HB2	1:A:265[C]:SER:OG	2.20	0.42
1:D:226[B]:GLU:HG2	3:D:644:HOH:O	2.19	0.42
1:J:44[B]:PRO:HD2	3:J:605:HOH:O	2.20	0.42
1:A:1[C]:MET:SD	1:D:118:THR:HB	2.60	0.41
1:G:339[B]:SER:OG	3:G:501:HOH:O	2.21	0.41
1:J:195:GLN:HG2	3:J:794:HOH:O	2.19	0.41
1:J:26:PRO:HA	1:J:27:GLY:HA2	1.67	0.41
1:D:361[B]:LEU:HD22	1:D:367:VAL:HB	2.02	0.41
1:D:155[A]:HIS:HB3	3:D:620:HOH:O	2.21	0.41
1:D:44[B]:PRO:HD2	3:D:672:HOH:O	2.19	0.41
1:D:31:LEU:HD11	1:D:388[A]:LEU:HD21	2.02	0.41
1:J:134[B]:LYS:HA	1:J:144:VAL:HG21	2.04	0.40
1:A:254:ARG:HG2	1:D:287:PRO:HA	2.02	0.40
1:D:122[A]:ARG:NH1	1:D:170:GLN:OE1	2.54	0.40

All (2) 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)
3:D:609:HOH:O	3:G:727:HOH:O[1_556]	2.01	0.19
3:G:841:HOH:O	3:J:538:HOH:O[1_455]	2.02	0.18

## 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	451/396 (114%)	438 (97%)	13 (3%)	0	100	100
1	D	453/396 (114%)	432 (95%)	18 (4%)	3 (1%)	22	10
1	G	452/396 (114%)	439 (97%)	12 (3%)	1 (0%)	47	33
1	J	447/396 (113%)	434 (97%)	12 (3%)	1 (0%)	47	33
All	All	1803/1584 (114%)	1743 (97%)	55 (3%)	5 (0%)	41	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	335	ASN
1	D	336	ARG
1	G	16	LEU
1	J	337	ASP
1	D	337	ASP

### 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	379/320 (118%)	369 (97%)	10 (3%)	46	32
1	D	381/320 (119%)	371 (97%)	10 (3%)	46	32
1	G	380/320 (119%)	368 (97%)	12 (3%)	39	25
1	J	375/320 (117%)	365 (97%)	10 (3%)	44	31
All	All	1515/1280 (118%)	1473 (97%)	42 (3%)	62	30

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165[A]	SER
1	A	165[B]	SER
1	A	212[A]	PHE

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Mol	Chain	Res	Type
1	A	212[B]	PHE
1	A	324[A]	LEU
1	A	324[B]	LEU
1	A	360[A]	ARG
1	A	360[B]	ARG
1	A	388[A]	LEU
1	A	388[B]	LEU
1	D	155[A]	HIS
1	D	155[B]	HIS
1	D	212[A]	PHE
1	D	212[B]	PHE
1	D	324[A]	LEU
1	D	324[B]	LEU
1	D	360[A]	ARG
1	D	360[B]	ARG
1	D	388[A]	LEU
1	D	388[B]	LEU
1	G	116[A]	LYS
1	G	116[B]	LYS
1	G	165[A]	SER
1	G	165[B]	SER
1	G	212[A]	PHE
1	G	212[B]	PHE
1	G	324[A]	LEU
1	G	324[B]	LEU
1	G	360[A]	ARG
1	G	360[B]	ARG
1	G	388[A]	LEU
1	G	388[B]	LEU
1	J	122[A]	ARG
1	J	122[B]	ARG
1	J	165[A]	SER
1	J	165[B]	SER
1	J	212[A]	PHE
1	J	212[B]	PHE
1	J	360[A]	ARG
1	J	360[B]	ARG
1	J	388[A]	LEU
1	J	388[B]	LEU

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

Mol	Chain	Res	Type
1	D	330	GLN
1	J	235	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](#)

4 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	PMP	D	401	-	16,16,16	0.80	0	21,23,23	1.75	3 (14%)
2	PMP	J	401	-	16,16,16	0.95	2 (12%)	21,23,23	1.59	5 (23%)
2	PMP	A	401	-	16,16,16	0.87	1 (6%)	21,23,23	1.33	3 (14%)
2	PMP	G	401	-	16,16,16	0.97	2 (12%)	21,23,23	1.47	2 (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	PMP	D	401	-	-	3/8/8/8	0/1/1/1
2	PMP	J	401	-	-	2/8/8/8	0/1/1/1
2	PMP	A	401	-	-	0/8/8/8	0/1/1/1
2	PMP	G	401	-	-	2/8/8/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	PMP	C2-N1	2.59	1.38	1.33
2	J	401	PMP	C2-N1	2.58	1.38	1.33
2	A	401	PMP	C2-N1	2.04	1.37	1.33
2	J	401	PMP	C3-C2	-2.01	1.38	1.40
2	G	401	PMP	C3-C2	-2.00	1.38	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PMP	C6-C5-C4	5.30	121.87	118.12
2	G	401	PMP	C6-C5-C4	4.67	121.42	118.12
2	D	401	PMP	C5-C6-N1	-3.72	117.62	123.82
2	G	401	PMP	C5-C6-N1	-3.30	118.32	123.82
2	J	401	PMP	C5-C6-N1	-3.28	118.36	123.82
2	A	401	PMP	C6-C5-C4	2.98	120.22	118.12
2	A	401	PMP	C5-C6-N1	-2.52	119.62	123.82
2	J	401	PMP	C6-C5-C4	2.42	119.83	118.12
2	J	401	PMP	O4P-P-O1P	2.41	113.22	106.47
2	D	401	PMP	C5A-C5-C6	-2.40	115.43	119.37
2	J	401	PMP	C6-N1-C2	2.24	123.31	119.17
2	A	401	PMP	O3P-P-O4P	2.18	112.54	106.73
2	J	401	PMP	C2A-C2-N1	2.07	121.71	117.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	PMP	C5A-O4P-P-O2P
2	J	401	PMP	C5A-O4P-P-O2P
2	J	401	PMP	C5A-O4P-P-O3P
2	G	401	PMP	C5A-O4P-P-O2P
2	D	401	PMP	C5A-O4P-P-O3P
2	G	401	PMP	C5A-O4P-P-O3P
2	D	401	PMP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PMP	2	0
2	J	401	PMP	2	0
2	A	401	PMP	2	0
2	G	401	PMP	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	396/396 (100%)	-0.47	5 (1%) 77 74	18, 27, 46, 70	0
1	D	396/396 (100%)	-0.41	10 (2%) 57 52	18, 27, 49, 88	0
1	G	396/396 (100%)	-0.41	9 (2%) 60 56	17, 27, 49, 77	0
1	J	396/396 (100%)	-0.37	11 (2%) 53 47	18, 27, 50, 73	0
All	All	1584/1584 (100%)	-0.41	35 (2%) 62 57	17, 27, 48, 88	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	331[A]	GLU	9.8
1	J	10	ALA	7.4
1	D	336	ARG	7.3
1	J	26	PRO	6.2
1	A	10	ALA	5.6
1	D	14	LEU	5.5
1	D	330	GLN	5.4
1	J	14	LEU	4.7
1	G	26	PRO	4.5
1	J	24	GLU	4.4
1	A	14	LEU	4.3
1	A	26	PRO	4.2
1	G	335	ASN	3.8
1	G	24	GLU	3.6
1	J	20	PHE	3.5
1	D	332	LYS	3.4
1	G	10	ALA	3.3
1	D	334	ALA	3.3
1	D	333	GLY	3.2
1	J	27	GLY	3.2
1	D	26	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	27	GLY	3.1
1	D	335	ASN	3.1
1	A	335	ASN	3.0
1	G	21	ARG	2.5
1	A	21	ARG	2.4
1	J	335	ASN	2.4
1	G	14	LEU	2.3
1	J	16	LEU	2.3
1	J	19	LEU	2.3
1	J	343[A]	LYS	2.3
1	G	20	PHE	2.2
1	D	10	ALA	2.2
1	J	25	ARG	2.2
1	G	19	LEU	2.1

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PMP	A	401	16/16	0.98	0.06	20,23,26,29	0
2	PMP	J	401	16/16	0.99	0.07	19,21,25,31	0
2	PMP	D	401	16/16	0.99	0.07	17,22,26,31	0
2	PMP	G	401	16/16	0.99	0.08	19,22,25,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.