



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:10 AM GMT

PDB ID : 2AA3  
Title : Crystal structure of Plasmodium vivax lactate dehydrogenase complex with APADH  
Authors : Chaikuad, A.; Fairweather, V.; Conners, R.; Joseph-Horne, T.; Turgut-Balik, D.; Brady, R.L.  
Deposited on : 2005-07-13  
Resolution : 2.05 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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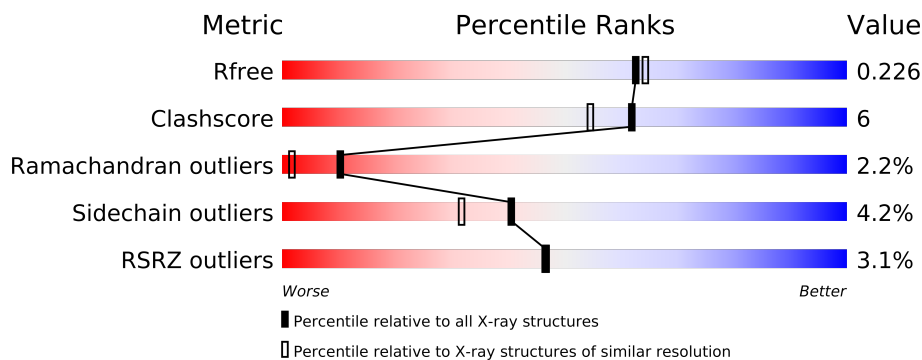
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.05 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))
$R_{free}$	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	
1	C	321	
1	D	321	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10302 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	106	1	0
			2408	1540	403	451	14			
1	B	315	Total	C	N	O	S	34	1	0
			2398	1534	400	450	14			
1	C	318	Total	C	N	O	S	118	2	0
			2433	1557	409	453	14			
1	D	315	Total	C	N	O	S	125	1	0
			2398	1534	400	450	14			

There are 24 discrepancies between the modelled and reference sequences:

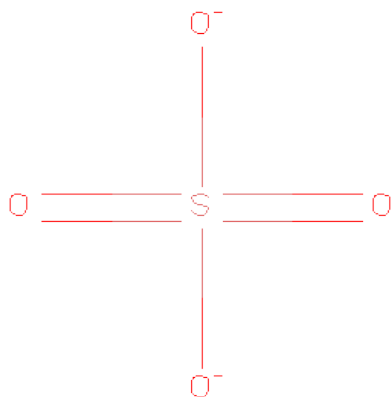
Chain	Residue	Modelled	Actual	Comment	Reference
A	330	HIS	-	EXPRESSION TAG	GB 66967948
A	331	HIS	-	EXPRESSION TAG	GB 66967948
A	332	HIS	-	EXPRESSION TAG	GB 66967948
A	333	HIS	-	EXPRESSION TAG	GB 66967948
A	334	HIS	-	EXPRESSION TAG	GB 66967948
A	335	HIS	-	EXPRESSION TAG	GB 66967948
B	330	HIS	-	EXPRESSION TAG	GB 66967948
B	331	HIS	-	EXPRESSION TAG	GB 66967948
B	332	HIS	-	EXPRESSION TAG	GB 66967948
B	333	HIS	-	EXPRESSION TAG	GB 66967948
B	334	HIS	-	EXPRESSION TAG	GB 66967948
B	335	HIS	-	EXPRESSION TAG	GB 66967948
C	330	HIS	-	EXPRESSION TAG	GB 66967948
C	331	HIS	-	EXPRESSION TAG	GB 66967948
C	332	HIS	-	EXPRESSION TAG	GB 66967948
C	333	HIS	-	EXPRESSION TAG	GB 66967948
C	334	HIS	-	EXPRESSION TAG	GB 66967948
C	335	HIS	-	EXPRESSION TAG	GB 66967948
D	330	HIS	-	EXPRESSION TAG	GB 66967948
D	331	HIS	-	EXPRESSION TAG	GB 66967948
D	332	HIS	-	EXPRESSION TAG	GB 66967948

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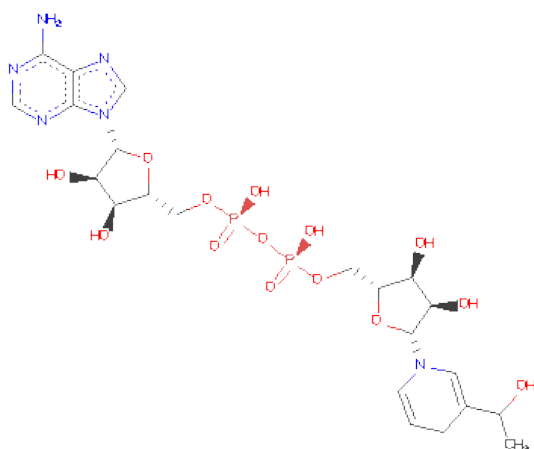
Chain	Residue	Modelled	Actual	Comment	Reference
D	333	HIS	-	EXPRESSION TAG	GB 66967948
D	334	HIS	-	EXPRESSION TAG	GB 66967948
D	335	HIS	-	EXPRESSION TAG	GB 66967948

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETYL PYRIDINE ADENINE DINUCLEOTIDE, REDUCED (three-letter code: AP0) (formula: C<sub>22</sub>H<sub>32</sub>N<sub>6</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	22	6	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	22	6	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	22	6	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	22	6	14	2		

- Molecule 4 is water.

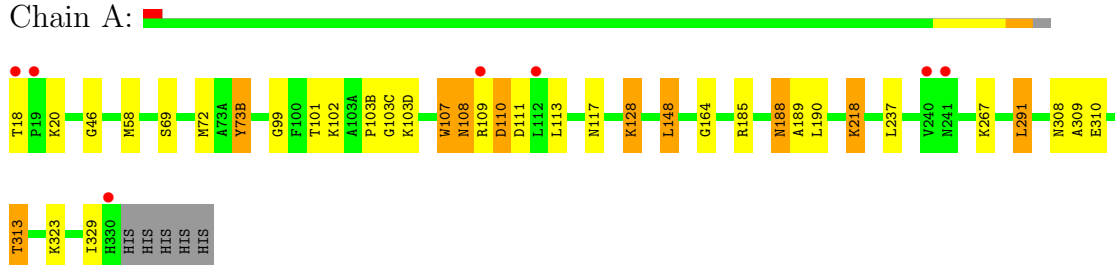
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	121	Total	O	0	0
			121	121		
4	C	121	Total	O	0	0
			121	121		
4	D	88	Total	O	0	0
			88	88		

### 3 Residue-property plots

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

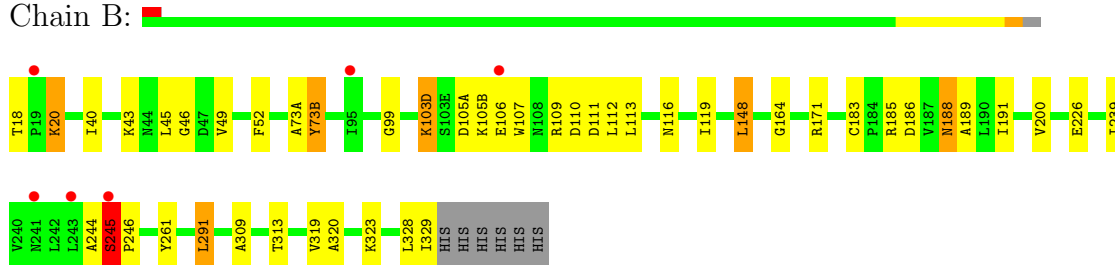
- Molecule 1: L-lactate dehydrogenase

Chain A:



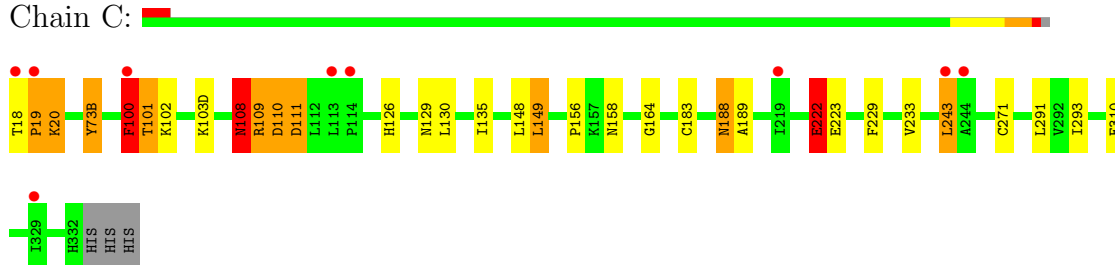
- Molecule 1: L-lactate dehydrogenase

Chain B:



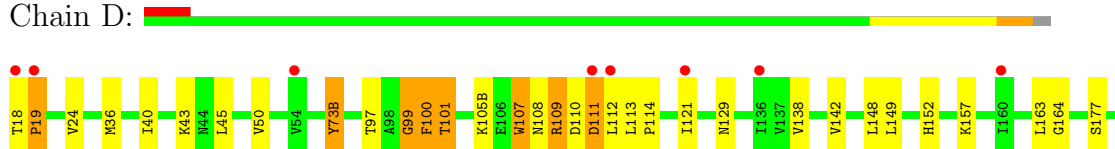
- Molecule 1: L-lactate dehydrogenase

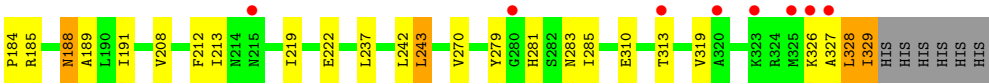
Chain C:



- Molecule 1: L-lactate dehydrogenase

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.48Å 128.45Å 130.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.67 – 2.05 29.14 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.3 (91.67-2.05) 98.4 (29.14-2.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.191 , 0.226 0.192 , 0.226	Depositor DCC
$R_{free}$ test set	4276 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.6	EDS
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 85446 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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: AP0, SO4

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	1.06	4/2448 (0.2%)	0.85	4/3315 (0.1%)
1	B	1.00	4/2437 (0.2%)	0.92	10/3300 (0.3%)
1	C	0.99	3/2478 (0.1%)	0.88	12/3356 (0.4%)
1	D	0.86	3/2437 (0.1%)	0.77	2/3300 (0.1%)
All	All	0.98	14/9800 (0.1%)	0.86	28/13271 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	2	1
1	D	1	2
All	All	3	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	LYS	CE-NZ	15.30	1.87	1.49
1	C	222	GLU	CD-OE1	14.62	1.41	1.25
1	A	128	LYS	CE-NZ	14.36	1.84	1.49
1	C	222	GLU	CD-OE2	12.60	1.39	1.25
1	B	226	GLU	CD-OE1	12.25	1.39	1.25
1	B	226	GLU	CD-OE2	10.85	1.37	1.25
1	D	222	GLU	CD-OE2	8.96	1.35	1.25
1	A	218	LYS	CD-CE	8.42	1.72	1.51
1	A	323	LYS	CD-CE	7.72	1.70	1.51
1	B	107	TRP	CA-CB	6.84	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	ASP	CA-CB	5.81	1.66	1.53
1	B	185	ARG	CG-CD	-5.70	1.37	1.51
1	D	222	GLU	CD-OE1	5.57	1.31	1.25
1	D	100	PHE	N-CA	5.36	1.57	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	GLU	CA-CB-CG	15.37	147.21	113.40
1	C	100	PHE	O-C-N	14.45	145.82	122.70
1	C	100	PHE	CA-C-N	-9.95	95.32	117.20
1	A	218	LYS	CD-CE-NZ	-9.86	89.02	111.70
1	B	107	TRP	CB-CA-C	-9.71	90.97	110.40
1	C	110	ASP	O-C-N	-8.73	108.74	122.70
1	A	291	LEU	CA-CB-CG	8.33	134.47	115.30
1	B	291	LEU	CA-CB-CG	8.00	133.70	115.30
1	C	100	PHE	C-N-CA	-7.79	102.23	121.70
1	C	110	ASP	CB-CA-C	-7.73	94.95	110.40
1	D	100	PHE	N-CA-C	7.58	131.46	111.00
1	B	112	LEU	CA-CB-CG	7.23	131.93	115.30
1	B	106	GLU	CB-CG-CD	7.07	133.28	114.20
1	B	171	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	C	110	ASP	CA-C-N	6.46	131.41	117.20
1	A	99	GLY	O-C-N	6.27	132.73	122.70
1	B	107	TRP	N-CA-CB	-5.91	99.97	110.60
1	B	185	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	110	ASP	N-CA-CB	-5.59	100.53	110.60
1	D	111	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	99	GLY	CA-C-N	-5.48	105.14	117.20
1	B	245	SER	N-CA-CB	5.40	118.60	110.50
1	B	105(A)	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	110	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	111	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	243[A]	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	243[B]	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	222	GLU	OE1-CD-OE2	5.03	129.34	123.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	101	THR	CB,CA
1	D	110	ASP	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TRP	Peptide
1	A	108	ASN	Peptide
1	B	244	ALA	Peptide
1	C	108	ASN	Peptide
1	D	99	GLY	Mainchain,Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2408	0	2505	33	0
1	B	2398	0	2498	29	0
1	C	2433	0	2530	31	0
1	D	2398	0	2497	33	0
2	A	5	0	0	0	0
2	C	5	0	0	1	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
4	A	149	0	0	1	0
4	B	121	0	0	1	0
4	C	121	0	0	2	0
4	D	88	0	0	0	0
All	All	10302	0	10134	109	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (109) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:LYS:CE	1:A:128:LYS:NZ	1.84	1.39
1:A:218:LYS:CE	1:A:218:LYS:NZ	1.87	1.37
1:D:18:THR:HA	1:D:19:PRO:O	1.27	1.27
1:A:109:ARG:HB2	1:A:110:ASP:HB3	1.33	1.08

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:18:THR:HA	1:D:19:PRO:C	1.66	1.06
1:D:326:LYS:O	1:D:329:ILE:HD13	1.58	1.04
1:B:239:ILE:HG22	1:B:245:SER:H	1.24	1.03
1:A:109:ARG:CB	1:A:110:ASP:HB3	1.91	1.00
1:B:319:VAL:HG12	1:B:323:LYS:HE2	1.47	0.94
1:A:109:ARG:HB2	1:A:110:ASP:CB	1.97	0.93
1:A:109:ARG:CB	1:A:110:ASP:CB	2.46	0.92
1:C:291:LEU:HD11	1:C:293:ILE:HD11	1.51	0.92
1:C:291:LEU:CD1	1:C:293:ILE:HD11	2.04	0.86
1:D:18:THR:CA	1:D:19:PRO:O	2.21	0.85
1:C:73(B)[B]:TYR:CD2	1:D:73(B)[B]:TYR:CD2	2.65	0.84
1:B:103(D):LYS:NZ	1:B:111:ASP:OD2	2.11	0.83
1:D:18:THR:CA	1:D:19:PRO:C	2.46	0.83
1:C:73(B)[B]:TYR:CE2	1:D:73(B)[B]:TYR:CD2	2.67	0.82
1:C:73(B)[B]:TYR:CD2	1:D:73(B)[B]:TYR:CE2	2.68	0.81
1:D:326:LYS:O	1:D:329:ILE:CD1	2.31	0.79
1:A:109:ARG:HB3	1:A:110:ASP:CB	2.13	0.78
1:C:126:HIS:HE1	4:C:1511:HOH:O	1.67	0.76
1:A:109:ARG:NH1	1:A:111:ASP:OD1	2.19	0.75
1:A:218:LYS:NZ	1:A:218:LYS:CD	2.52	0.72
1:A:20:LYS:HE3	1:A:46:GLY:HA2	1.72	0.71
1:C:291:LEU:CD1	1:C:293:ILE:CD1	2.68	0.70
1:B:320:ALA:HA	1:B:323:LYS:HE3	1.73	0.70
1:C:73(B)[B]:TYR:CE2	1:D:73(B)[B]:TYR:HD2	2.09	0.69
1:B:99:GLY:HA2	1:B:119:ILE:HD13	1.74	0.69
1:A:109:ARG:HB3	1:A:110:ASP:HB2	1.73	0.69
1:C:73(B)[B]:TYR:HD2	1:D:73(B)[B]:TYR:CE2	2.14	0.65
1:D:327:ALA:O	1:D:328:LEU:HB2	1.97	0.64
1:A:58:MET:HG2	1:C:243[B]:LEU:HD22	1.81	0.63
1:C:129:ASN:OD1	1:C:130:LEU:HG	2.01	0.61
1:A:128:LYS:CD	1:A:128:LYS:NZ	2.64	0.59
1:B:148:LEU:HD21	1:B:329:ILE:HD13	1.83	0.59
1:A:109:ARG:HB2	1:A:110:ASP:CA	2.33	0.58
1:D:113:LEU:N	1:D:114:PRO:CD	2.66	0.58
1:D:121:ILE:HG12	1:D:152:HIS:CE1	2.38	0.58
1:A:309:ALA:O	1:A:313:THR:HG23	2.03	0.58
1:B:110:ASP:HA	1:B:113:LEU:HD23	1.87	0.56
1:B:239:ILE:CG2	1:B:245:SER:H	2.09	0.56
1:A:109:ARG:HB3	1:A:110:ASP:HB3	1.78	0.55
1:D:188:ASN:HD22	1:D:189:ALA:H	1.53	0.55
1:C:310:GLU:OE2	2:C:1002:SO4:O1	2.25	0.54
1:B:20:LYS:HE3	1:B:46:GLY:HA2	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:183:CYS:HG	1:D:73(B)[A]:TYR:HE2	1.57	0.53
1:B:239:ILE:HG22	1:B:245:SER:N	2.08	0.53
1:A:73(B)[A]:TYR:HE2	1:C:183:CYS:HG	1.56	0.52
1:A:308:ASN:OD1	1:A:310:GLU:HG2	2.09	0.52
1:C:291:LEU:HD13	1:C:293:ILE:CD1	2.39	0.51
1:A:18:THR:HG21	4:A:1534:HOH:O	2.09	0.51
1:D:142:VAL:HG11	1:D:163:LEU:O	2.10	0.51
1:D:113:LEU:N	1:D:114:PRO:HD2	2.26	0.51
1:B:261:TYR:O	1:C:18:THR:HG23	2.12	0.50
1:C:188:ASN:HD22	1:C:189:ALA:H	1.59	0.50
1:A:109:ARG:CZ	1:A:111:ASP:OD1	2.60	0.49
1:B:188:ASN:HD22	1:B:189:ALA:H	1.61	0.49
1:D:24:VAL:HG22	1:D:50:VAL:HB	1.95	0.48
1:B:103(D):LYS:CE	1:B:111:ASP:OD2	2.61	0.48
1:C:222:GLU:HG2	1:C:223:GLU:N	2.27	0.48
1:D:242:LEU:O	1:D:243:LEU:HB2	2.13	0.48
1:B:103(D):LYS:HZ1	1:B:111:ASP:CG	2.16	0.48
1:C:19:PRO:O	1:C:20:LYS:O	2.32	0.48
1:B:73(A):ALA:O	1:B:73(B)[B]:TYR:HB2	2.14	0.48
1:D:138:VAL:O	3:D:1403:AP0:H2	2.14	0.47
1:A:73(B)[B]:TYR:CD1	1:B:73(B)[B]:TYR:CD2	3.03	0.46
1:C:156:PRO:HB2	1:C:158:ASN:OD1	2.15	0.46
1:B:116:ASN:HA	1:B:119:ILE:HD12	1.98	0.46
1:B:245:SER:HA	1:B:246:PRO:HD2	1.75	0.46
1:D:36:MET:O	1:D:40:ILE:HG13	2.16	0.46
1:A:188:ASN:HD22	1:A:189:ALA:H	1.63	0.46
1:D:310:GLU:O	1:D:313:THR:HG22	2.16	0.45
1:A:185:ARG:HD2	1:C:73(B)[B]:TYR:HD1	1.82	0.45
1:A:58:MET:HG2	1:C:243[B]:LEU:CD2	2.47	0.45
1:B:73(B)[B]:TYR:HE1	1:D:185:ARG:CZ	2.29	0.44
1:C:126:HIS:HD2	4:C:1508:HOH:O	1.99	0.44
1:A:73(B)[B]:TYR:HD1	1:B:73(B)[B]:TYR:CE2	2.35	0.44
1:D:279:TYR:O	1:D:281:HIS:CD2	2.71	0.44
1:C:100:PHE:CD2	1:C:100:PHE:N	2.85	0.44
1:C:229:PHE:O	1:C:233:VAL:HG23	2.17	0.44
1:D:208:VAL:HB	1:D:212:PHE:CE1	2.53	0.43
1:D:213:ILE:HA	1:D:219:ILE:O	2.18	0.43
1:C:100:PHE:HD2	1:C:100:PHE:N	2.16	0.43
1:C:271:CYS:HB2	1:C:291:LEU:HD21	2.00	0.43
1:D:285:ILE:HG12	1:D:319:VAL:HG13	2.01	0.43
1:B:111:ASP:HB2	4:B:1476:HOH:O	2.19	0.43
1:D:43:LYS:HB2	1:D:45:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:97:THR:HG22	1:D:138:VAL:HB	2.02	0.42
1:A:185:ARG:HD2	1:C:73(B)[B]:TYR:CD1	2.54	0.42
1:B:40:ILE:HG21	1:B:49:VAL:HG22	2.02	0.42
1:A:73(B)[B]:TYR:CD1	1:B:73(B)[B]:TYR:CE2	3.07	0.42
1:B:191:ILE:HA	1:B:200:VAL:O	2.20	0.42
1:B:309:ALA:O	1:B:313:THR:HG23	2.20	0.41
1:B:43:LYS:HB2	1:B:45:LEU:HG	2.02	0.41
1:D:191:ILE:O	1:D:270:VAL:HG11	2.21	0.41
1:D:177:SER:CB	1:D:184:PRO:HA	2.50	0.41
1:C:73(B)[B]:TYR:HE2	1:D:73(B)[B]:TYR:HD2	1.63	0.41
1:A:109:ARG:HD2	1:A:111:ASP:OD1	2.20	0.41
1:A:113:LEU:HB3	1:A:329:ILE:HD11	2.03	0.41
1:C:135:ILE:HG21	1:C:149:LEU:HD13	2.03	0.41
1:A:267:LYS:HA	1:B:186:ASP:OD2	2.21	0.41
1:C:291:LEU:HD13	1:C:293:ILE:HD13	2.02	0.41
3:D:1403:AP0:H2	3:D:1403:AP0:H81	1.83	0.41
1:A:69:SER:HA	1:A:72:MET:HE2	2.03	0.41
1:A:117:ASN:ND2	1:A:148:LEU:HG	2.35	0.40
1:B:52:PHE:CE2	3:B:1407:AP0:H111	2.56	0.40
1:C:243[B]:LEU:HA	1:C:243[B]:LEU:HD12	1.77	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	315/321 (98%)	296 (94%)	11 (4%)	8 (2%)	9	1
1	B	314/321 (98%)	302 (96%)	10 (3%)	2 (1%)	33	20
1	C	318/321 (99%)	294 (92%)	17 (5%)	7 (2%)	10	2
1	D	314/321 (98%)	291 (93%)	12 (4%)	11 (4%)	6	0
All	All	1261/1284 (98%)	1183 (94%)	50 (4%)	28 (2%)	10	2

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	LYS
1	A	103(C)	GLY
1	A	108	ASN
1	B	245	SER
1	C	20	LYS
1	C	101	THR
1	C	103(D)	LYS
1	C	109	ARG
1	D	19	PRO
1	D	100	PHE
1	D	111	ASP
1	D	112	LEU
1	D	328	LEU
1	A	103(D)	LYS
1	A	110	ASP
1	C	108	ASN
1	D	101	THR
1	D	107	TRP
1	D	108	ASN
1	D	99	GLY
1	D	109	ARG
1	D	164	GLY
1	A	164	GLY
1	C	164	GLY
1	A	103(B)	PRO
1	A	101	THR
1	B	164	GLY
1	C	19	PRO

### 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	269/273 (98%)	260 (97%)	9 (3%)	50	42
1	B	268/273 (98%)	256 (96%)	12 (4%)	38	28
1	C	272/273 (100%)	260 (96%)	12 (4%)	39	29
1	D	268/273 (98%)	252 (94%)	16 (6%)	27	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1077/1092 (99%)	1028 (96%)	49 (4%)	40	28

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73(B)[A]	TYR
1	A	73(B)[B]	TYR
1	A	107	TRP
1	A	148	LEU
1	A	188	ASN
1	A	190	LEU
1	A	237	LEU
1	A	291	LEU
1	A	313	THR
1	B	18	THR
1	B	20	LYS
1	B	73(B)[A]	TYR
1	B	73(B)[B]	TYR
1	B	103(D)	LYS
1	B	105(B)	LYS
1	B	109	ARG
1	B	148	LEU
1	B	188	ASN
1	B	245	SER
1	B	291	LEU
1	B	328	LEU
1	C	73(B)[A]	TYR
1	C	73(B)[B]	TYR
1	C	100	PHE
1	C	102	LYS
1	C	108	ASN
1	C	109	ARG
1	C	110	ASP
1	C	111	ASP
1	C	148	LEU
1	C	149	LEU
1	C	188	ASN
1	C	222	GLU
1	D	73(B)[A]	TYR
1	D	73(B)[B]	TYR
1	D	101	THR
1	D	105(B)	LYS

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Mol	Chain	Res	Type
1	D	107	TRP
1	D	109	ARG
1	D	110	ASP
1	D	129	ASN
1	D	148	LEU
1	D	149	LEU
1	D	157	LYS
1	D	188	ASN
1	D	237	LEU
1	D	243	LEU
1	D	283	ASN
1	D	329	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	117	ASN
1	A	132(B)	ASN
1	A	152	HIS
1	A	188	ASN
1	A	210(B)	GLN
1	A	234	ASN
1	A	306	GLN
1	B	140	ASN
1	B	152	HIS
1	B	188	ASN
1	B	210(B)	GLN
1	C	126	HIS
1	C	140	ASN
1	C	152	HIS
1	C	178	GLN
1	C	188	ASN
1	C	234	ASN
1	D	117	ASN
1	D	132(B)	ASN
1	D	152	HIS
1	D	178	GLN
1	D	188	ASN
1	D	210(B)	GLN
1	D	234	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	SO4	A	1001	-	4,4,4	0.43	0	6,6,6	0.55	0
3	AP0	A	1401	-	48,48,48	2.23	10 (20%)	73,73,73	2.46	19 (26%)
3	AP0	B	1407	-	48,48,48	1.99	10 (20%)	73,73,73	2.35	19 (26%)
2	SO4	C	1002	-	4,4,4	0.18	0	6,6,6	0.22	0
3	AP0	C	1405	-	48,48,48	1.97	11 (22%)	73,73,73	2.26	18 (24%)
3	AP0	D	1403	-	48,48,48	2.13	12 (25%)	73,73,73	2.36	23 (31%)

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	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	AP0	A	1401	-	3/3/13/16	0/30/72/72	0/3/5/5
3	AP0	B	1407	-	3/3/13/16	0/30/72/72	0/3/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	1002	-	-	0/0/0/0	0/0/0/0
3	AP0	C	1405	-	3/3/13/16	0/30/72/72	0/3/5/5
3	AP0	D	1403	-	3/3/13/16	0/30/72/72	0/3/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1403	AP0	O7N-C7N	-6.06	1.21	1.42
3	A	1401	AP0	O7N-C7N	-6.06	1.21	1.42
3	B	1407	AP0	O7N-C7N	-5.93	1.22	1.42
3	D	1403	AP0	C2N-C3N	5.93	1.40	1.33
3	D	1403	AP0	C2D-C1D	-5.91	1.33	1.53
3	A	1401	AP0	C2D-C1D	-5.76	1.34	1.53
3	A	1401	AP0	C2N-C3N	5.64	1.40	1.33
3	C	1405	AP0	C2N-C3N	5.44	1.40	1.33
3	B	1407	AP0	C2N-C3N	5.41	1.39	1.33
3	C	1405	AP0	O7N-C7N	-5.40	1.23	1.42
3	A	1401	AP0	O2D-C2D	-5.24	1.30	1.43
3	C	1405	AP0	C2D-C1D	-5.20	1.36	1.53
3	A	1401	AP0	C4N-C5N	-5.16	1.37	1.49
3	B	1407	AP0	C2D-C1D	-4.90	1.37	1.53
3	A	1401	AP0	C6N-C5N	4.28	1.42	1.33
3	D	1403	AP0	C1D-N1N	-4.22	1.36	1.46
3	B	1407	AP0	PN-O3	4.14	1.67	1.59
3	D	1403	AP0	O2D-C2D	-3.90	1.33	1.43
3	C	1405	AP0	O2D-C2D	-3.87	1.33	1.43
3	C	1405	AP0	C4N-C5N	-3.81	1.40	1.49
3	D	1403	AP0	C4N-C5N	-3.67	1.41	1.49
3	B	1407	AP0	C6N-C5N	3.63	1.41	1.33
3	B	1407	AP0	C4N-C5N	-3.44	1.41	1.49
3	D	1403	AP0	C6N-C5N	3.40	1.40	1.33
3	C	1405	AP0	C4A-N9A	-3.27	1.33	1.37
3	C	1405	AP0	C1D-N1N	-3.23	1.39	1.46
3	A	1401	AP0	C1D-N1N	-3.20	1.39	1.46
3	B	1407	AP0	C1D-N1N	-3.18	1.39	1.46
3	A	1401	AP0	C4A-N9A	-2.97	1.33	1.37
3	D	1403	AP0	PN-O3	2.94	1.65	1.59
3	A	1401	AP0	PN-O3	2.93	1.65	1.59
3	B	1407	AP0	O2D-C2D	-2.83	1.36	1.43
3	D	1403	AP0	C8N-C7N	-2.55	1.34	1.50
3	D	1403	AP0	C4N-C3N	-2.48	1.39	1.47
3	D	1403	AP0	O4B-C1B	2.47	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1405	AP0	C6N-C5N	2.41	1.38	1.33
3	C	1405	AP0	PA-O3	2.38	1.64	1.59
3	B	1407	AP0	C8N-C7N	-2.34	1.36	1.50
3	C	1405	AP0	C4N-C3N	-2.26	1.40	1.47
3	D	1403	AP0	C7N-C3N	-2.18	1.48	1.51
3	C	1405	AP0	C8N-C7N	-2.13	1.37	1.50
3	B	1407	AP0	PA-O3	2.11	1.63	1.59
3	A	1401	AP0	C4N-C3N	-2.04	1.41	1.47

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401	AP0	N3A-C2A-N1A	-8.85	121.31	128.71
3	D	1403	AP0	N3A-C2A-N1A	-8.46	121.63	128.71
3	C	1405	AP0	N3A-C2A-N1A	-8.36	121.72	128.71
3	A	1401	AP0	C2D-C1D-N1N	7.65	132.71	113.21
3	B	1407	AP0	N3A-C2A-N1A	-7.52	122.42	128.71
3	B	1407	AP0	C2D-C1D-N1N	7.20	131.57	113.21
3	C	1405	AP0	C2D-C1D-N1N	7.17	131.48	113.21
3	D	1403	AP0	O4B-C1B-N9A	6.48	114.46	108.44
3	A	1401	AP0	C3D-C2D-C1D	6.43	114.13	101.35
3	A	1401	AP0	C8N-C7N-C3N	6.35	123.45	113.16
3	D	1403	AP0	O4D-C1D-N1N	6.07	120.90	108.05
3	A	1401	AP0	O2D-C2D-C1D	5.71	129.49	110.04
3	C	1405	AP0	O2D-C2D-C1D	5.70	129.45	110.04
3	D	1403	AP0	C2D-C1D-N1N	5.62	127.54	113.21
3	B	1407	AP0	C8N-C7N-C3N	5.49	122.05	113.16
3	C	1405	AP0	C3D-C2D-C1D	5.23	111.74	101.35
3	B	1407	AP0	O2D-C2D-C1D	5.11	127.42	110.04
3	B	1407	AP0	O4B-C1B-N9A	5.07	113.16	108.44
3	D	1403	AP0	C3D-C2D-C1D	5.04	111.36	101.35
3	D	1403	AP0	C8N-C7N-C3N	4.90	121.09	113.16
3	D	1403	AP0	O2D-C2D-C1D	4.74	126.16	110.04
3	B	1407	AP0	N3A-C4A-N9A	4.70	133.92	125.43
3	A	1401	AP0	O4D-C1D-N1N	4.55	117.68	108.05
3	A	1401	AP0	O3D-C3D-C2D	-4.54	97.05	111.83
3	C	1405	AP0	O4D-C1D-N1N	4.39	117.34	108.05
3	B	1407	AP0	O4D-C1D-N1N	4.26	117.07	108.05
3	B	1407	AP0	C3D-C2D-C1D	4.22	109.73	101.35
3	C	1405	AP0	O4B-C1B-N9A	4.13	112.29	108.44
3	A	1401	AP0	O4B-C1B-N9A	4.09	112.25	108.44
3	B	1407	AP0	C4N-C3N-C2N	-4.02	117.75	122.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1407	AP0	C4B-O4B-C1B	-4.00	105.40	109.75
3	C	1405	AP0	C8N-C7N-C3N	3.78	119.28	113.16
3	A	1401	AP0	C1B-N9A-C4A	-3.74	120.17	126.64
3	C	1405	AP0	N3A-C4A-N9A	3.69	132.10	125.43
3	D	1403	AP0	N3A-C4A-N9A	3.66	132.04	125.43
3	A	1401	AP0	C4N-C5N-C6N	-3.41	116.36	122.61
3	C	1405	AP0	O4B-C1B-C2B	-3.34	101.65	106.77
3	A	1401	AP0	O7N-C7N-C8N	3.31	123.93	110.58
3	D	1403	AP0	O2D-C2D-C3D	3.27	122.48	111.83
3	B	1407	AP0	O2D-C2D-C3D	3.27	122.47	111.83
3	D	1403	AP0	C4B-O4B-C1B	-3.25	106.22	109.75
3	B	1407	AP0	O3D-C3D-C2D	-3.23	101.34	111.83
3	D	1403	AP0	C4A-C5A-N7A	-3.21	106.78	109.52
3	C	1405	AP0	O7N-C7N-C8N	3.16	123.31	110.58
3	A	1401	AP0	N3A-C4A-N9A	3.13	131.08	125.43
3	D	1403	AP0	O3D-C3D-C2D	-3.01	102.04	111.83
3	A	1401	AP0	C4A-C5A-N7A	-2.96	106.98	109.52
3	B	1407	AP0	C5N-C4N-C3N	2.94	120.31	114.42
3	B	1407	AP0	C5A-C4A-N3A	-2.88	119.43	125.70
3	D	1403	AP0	O7N-C7N-C8N	2.78	121.79	110.58
3	D	1403	AP0	C5A-C4A-N3A	-2.78	119.64	125.70
3	D	1403	AP0	C5N-C4N-C3N	2.76	119.95	114.42
3	C	1405	AP0	O3D-C3D-C2D	-2.73	102.94	111.83
3	C	1405	AP0	C1B-N9A-C4A	-2.67	122.03	126.64
3	B	1407	AP0	C8A-N9A-C4A	2.62	108.90	106.90
3	A	1401	AP0	C8A-N9A-C1B	2.52	131.34	126.38
3	C	1405	AP0	C5A-C4A-N3A	-2.46	120.34	125.70
3	A	1401	AP0	C5N-C4N-C3N	2.44	119.31	114.42
3	A	1401	AP0	C2A-N1A-C6A	2.44	123.18	118.77
3	C	1405	AP0	C1D-N1N-C6N	-2.39	115.50	120.79
3	C	1405	AP0	C5N-C4N-C3N	2.38	119.19	114.42
3	B	1407	AP0	O7N-C7N-C3N	2.36	119.31	110.26
3	D	1403	AP0	C2A-N3A-C4A	2.29	120.53	114.01
3	D	1403	AP0	C4N-C5N-C6N	-2.28	118.42	122.61
3	A	1401	AP0	O2N-PN-O1N	2.25	124.80	112.21
3	B	1407	AP0	O4B-C1B-C2B	-2.25	103.33	106.77
3	A	1401	AP0	C5A-C4A-N3A	-2.20	120.91	125.70
3	B	1407	AP0	C4A-C5A-N7A	-2.19	107.64	109.52
3	D	1403	AP0	O2N-PN-O1N	2.15	124.21	112.21
3	C	1405	AP0	C4N-C5N-C6N	-2.13	118.70	122.61
3	C	1405	AP0	O2D-C2D-C3D	2.13	118.76	111.83
3	D	1403	AP0	C6N-N1N-C2N	2.12	122.22	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1403	AP0	C1D-N1N-C6N	-2.12	116.10	120.79
3	A	1401	AP0	N7A-C8A-N9A	-2.06	108.54	114.36
3	D	1403	AP0	C1B-N9A-C4A	-2.05	123.10	126.64
3	D	1403	AP0	N7A-C8A-N9A	-2.03	108.62	114.36
3	D	1403	AP0	C4N-C3N-C2N	-2.02	119.89	122.04
3	C	1405	AP0	C2A-N3A-C4A	2.02	119.75	114.01
3	B	1407	AP0	C4N-C5N-C6N	-2.00	118.93	122.61

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1407	AP0	C7N
3	B	1407	AP0	C1D
3	B	1407	AP0	C2D
3	C	1405	AP0	C7N
3	C	1405	AP0	C1D
3	C	1405	AP0	C2D
3	D	1403	AP0	C7N
3	D	1403	AP0	C1D
3	D	1403	AP0	C2D
3	A	1401	AP0	C7N
3	A	1401	AP0	C1D
3	A	1401	AP0	C2D

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	303/321 (94%)	-0.14	7 (2%) 57 58	9, 17, 29, 43	19 (6%)
1	B	315/321 (98%)	-0.01	6 (1%) 64 65	11, 19, 34, 47	32 (10%)
1	C	304/321 (94%)	-0.10	9 (2%) 48 48	9, 20, 30, 42	36 (11%)
1	D	300/321 (93%)	0.24	16 (5%) 25 24	12, 24, 39, 49	40 (13%)
All	All	1222/1284 (95%)	-0.00	38 (3%) 47 46	9, 20, 36, 49	127 (10%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	112	LEU	9.4
1	D	18	THR	8.0
1	A	18	THR	6.3
1	C	18	THR	4.7
1	D	111	ASP	4.3
1	A	330	HIS	4.3
1	B	19	PRO	4.0
1	C	244	ALA	3.8
1	D	326	LYS	3.5
1	C	100	PHE	3.4
1	D	323	LYS	3.4
1	A	109	ARG	3.0
1	D	280	GLY	2.9
1	A	112	LEU	2.9
1	D	215	ASN	2.9
1	C	243[A]	LEU	2.8
1	B	95	ILE	2.8
1	B	243	LEU	2.8
1	D	327	ALA	2.8
1	D	313	THR	2.6
1	C	19	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	113	LEU	2.5
1	C	329	ILE	2.5
1	D	136	ILE	2.4
1	D	19	PRO	2.4
1	D	121	ILE	2.4
1	D	160	ILE	2.4
1	C	114	PRO	2.3
1	C	219	ILE	2.3
1	D	325	MET	2.3
1	B	245	SER	2.2
1	B	106	GLU	2.2
1	A	19	PRO	2.2
1	D	54	VAL	2.2
1	B	241	ASN	2.1
1	A	240	VAL	2.1
1	D	320	ALA	2.0
1	A	241	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	SO4	C	1002	5/5	0.23	-	35,38,39,40	5
3	AP0	B	1407	44/44	0.11	-	17,23,34,36	0
3	AP0	C	1405	44/44	0.10	-	14,22,28,33	0
2	SO4	A	1001	5/5	0.13	-	29,29,31,32	5

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AP0	D	1403	44/44	0.12	-	24,31,38,39	0
3	AP0	A	1401	44/44	0.09	-	14,19,27,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.