



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:06 am GMT

PDB ID : 1QMG  
Title : ACETOHYDROXYACID ISOMEROREDUCTASE COMPLEXED WITH ITS REACTION PRODUCT DIHYDROXY-METHYLVALERATE, MANGANESE AND ADP-RIBOSE.  
Authors : Thomazeau, K.; Dumas, R.; Halgand, F.; Douce, R.; Biou, V.  
Deposited on : 1999-09-28  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

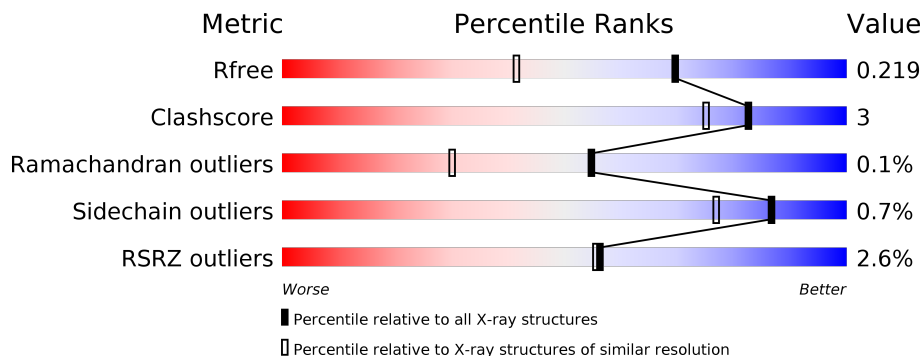
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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	524	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>
1	B	524	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	524	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	524	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	APX	A	600	X	-	-	-
2	APX	B	600	X	-	-	-
2	APX	C	600	X	-	-	-
2	APX	D	600	X	-	-	-
4	SO4	A	603	-	-	-	X
5	DMV	A	620	-	-	-	X
5	DMV	B	620	-	-	-	X
5	DMV	D	620	-	-	-	X

## 2 Entry composition i

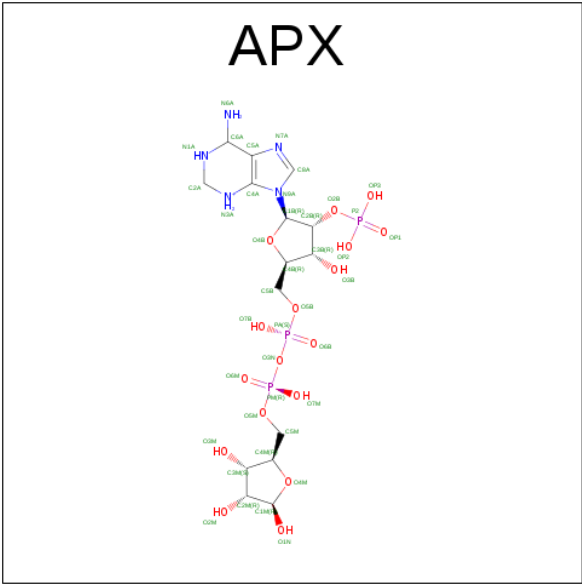
There are 6 unique types of molecules in this entry. The entry contains 18045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETOHYDROXY-ACID ISOMEROREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	4	0
			3948	2498	671	761	18			
1	B	510	Total	C	N	O	S	0	5	0
			3925	2485	667	754	19			
1	C	512	Total	C	N	O	S	0	4	0
			3936	2491	669	757	19			
1	D	513	Total	C	N	O	S	0	0	0
			3934	2491	670	755	18			

- Molecule 2 is 2'-MONOPHOSPHOADENOSINE-5'-DIPHOSPHORIBOSE (three-letter code: APX) (formula: C<sub>15</sub>H<sub>29</sub>N<sub>5</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			40	15	5	17	3	
2	B	1	Total	C	N	O	P	0
			40	15	5	17	3	

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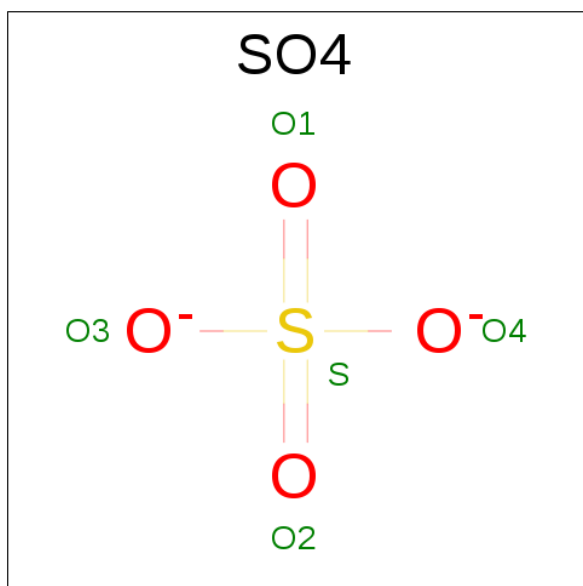
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			40	15	5	17	3		
2	D	1	Total	C	N	O	P	0	0
			40	15	5	17	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

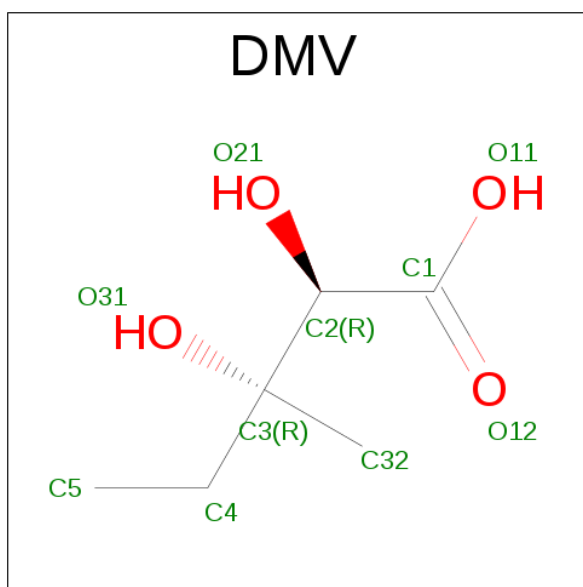
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		
3	D	2	Total	Mn	0	0
			2	2		
3	C	2	Total	Mn	0	0
			2	2		

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



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

- Molecule 5 is 2,3-DIHYDROXY-VALERIANIC ACID (three-letter code: DMV) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

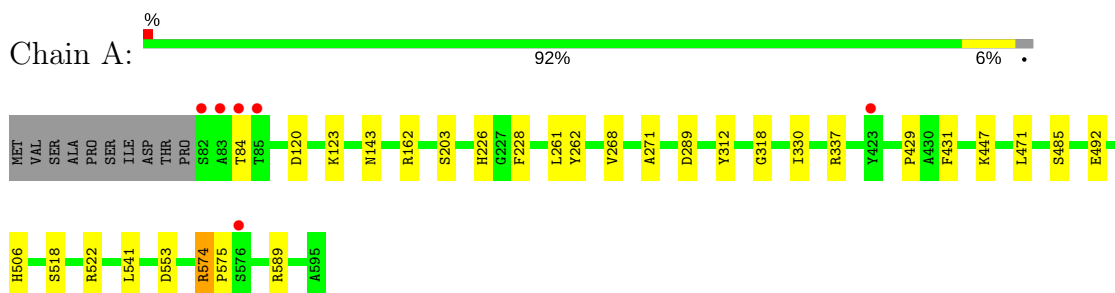
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	675	Total	O	0	0
			675	675		
6	B	538	Total	O	0	0
			538	538		
6	C	463	Total	O	0	0
			463	463		
6	D	413	Total	O	0	0
			413	413		

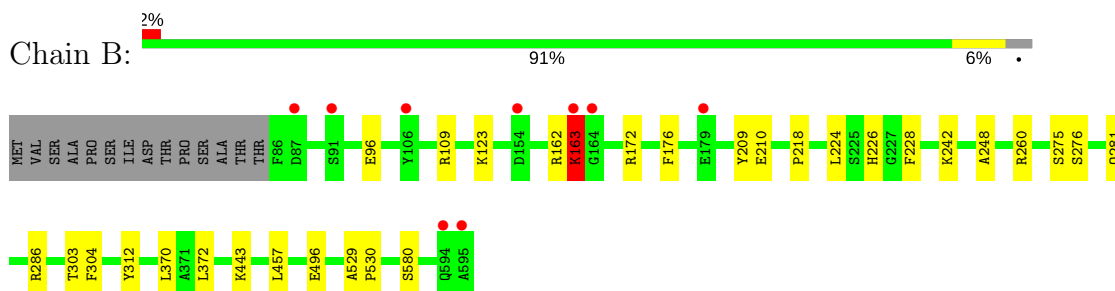
### 3 Residue-property plots

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

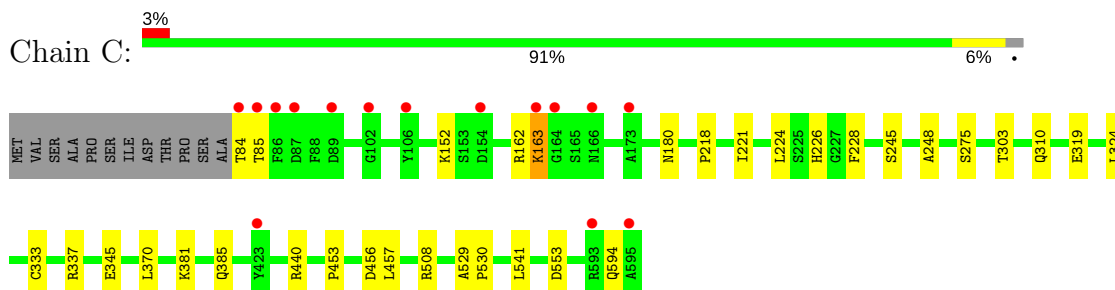
#### • Molecule 1: ACETOHYDROXY-ACID ISOMEROREDUCTASE



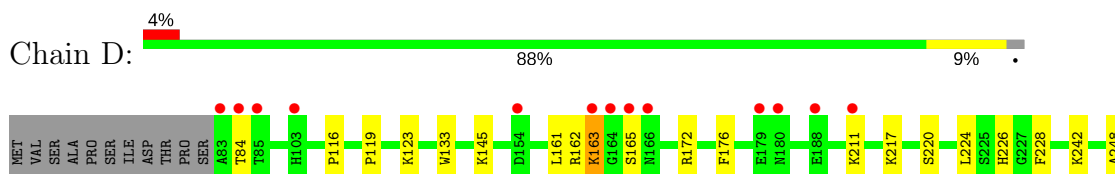
#### • Molecule 1: ACETOHYDROXY-ACID ISOMEROREDUCTASE



#### • Molecule 1: ACETOHYDROXY-ACID ISOMEROREDUCTASE



#### • Molecule 1: ACETOHYDROXY-ACID ISOMEROREDUCTASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.80Å 61.20Å 161.70Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60 10.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (10.00-1.60) 97.4 (10.00-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.16 (at 1.60Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.196 , 0.224 0.188 , 0.219	Depositor DCC
$R_{free}$ test set	13877 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 69.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: APX, MN, SO4, DMV

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	0.47	0/4043	0.65	1/5466 (0.0%)
1	B	0.44	0/4024	0.64	0/5439
1	C	0.43	0/4032	0.65	2/5451 (0.0%)
1	D	0.42	0/4013	0.60	0/5426
All	All	0.44	0/16112	0.63	3/21782 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	333[A]	CYS	CA-CB-SG	9.20	130.56	114.00
1	C	333[B]	CYS	CA-CB-SG	9.20	130.56	114.00
1	A	574	ARG	NE-CZ-NH2	7.09	123.85	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3948	0	3905	24	0
1	B	3925	0	3882	22	0
1	C	3936	0	3895	19	0
1	D	3934	0	3896	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	0	22	1	0
2	B	40	0	22	2	0
2	C	40	0	22	0	0
2	D	40	0	22	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	5	0	0	1	0
5	A	10	0	9	0	0
5	B	10	0	9	1	0
5	C	10	0	9	0	0
5	D	10	0	9	1	0
6	A	675	0	0	11	0
6	B	538	0	0	4	0
6	C	463	0	0	4	0
6	D	413	0	0	6	0
All	All	18045	0	15702	93	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 3.

All (93) 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:A:143:ASN:HB3	6:A:2310:HOH:O	1.69	0.93
1:C:162:ARG:HG2	6:C:2449:HOH:O	1.83	0.79
1:B:162:ARG:HG2	6:B:2531:HOH:O	1.85	0.75
1:B:218:PRO:HG3	6:B:2187:HOH:O	1.89	0.73
1:D:162:ARG:HG2	6:D:2072:HOH:O	1.87	0.73
1:D:123:LYS:HE2	1:D:286:ARG:HG2	1.76	0.68
1:C:163:LYS:HG2	6:C:2077:HOH:O	1.96	0.65
6:A:2285:HOH:O	1:C:218:PRO:HG3	1.96	0.64
1:D:574:ARG:HD3	6:D:2383:HOH:O	2.00	0.62
1:C:337:ARG:HD2	1:C:541:LEU:HD13	1.83	0.61
1:A:162:ARG:HB3	2:A:600:APX:H2A	1.84	0.60
1:A:447:LYS:HE3	6:A:2491:HOH:O	2.02	0.59
1:D:163:LYS:H	1:D:163:LYS:HD3	1.66	0.59
1:D:211:LYS:HG3	6:D:2102:HOH:O	2.03	0.59
1:C:152:LYS:HE2	6:C:2066:HOH:O	2.02	0.58
1:A:226:HIS:CD2	1:A:228:PHE:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:HB2	6:A:2442:HOH:O	2.05	0.56
1:D:571:ALA:O	1:D:574:ARG:HG2	2.05	0.56
1:D:242:LYS:HD3	6:D:2134:HOH:O	2.06	0.56
1:D:226:HIS:CD2	1:D:228:PHE:HB2	2.41	0.56
1:A:337:ARG:HD2	1:A:541:LEU:HD13	1.88	0.55
1:C:226:HIS:CD2	1:C:228:PHE:HB2	2.42	0.55
1:D:133:TRP:HB2	1:D:161:LEU:HD21	1.89	0.54
1:D:217:LYS:HG3	1:D:220:SER:HB3	1.88	0.54
1:C:453:PRO:HG2	1:C:456:ASP:HB2	1.91	0.53
1:A:262:TYR:CD1	6:A:2310:HOH:O	2.61	0.53
1:C:381:LYS:O	1:C:385:GLN:HG3	2.08	0.53
1:A:447:LYS:HE2	1:A:447:LYS:HA	1.90	0.52
1:B:172:ARG:HA	1:B:176:PHE:O	2.08	0.52
1:A:429:PRO:HG2	1:A:431:PHE:CZ	2.45	0.51
1:A:506:HIS:HE1	4:A:603:SO4:O3	1.92	0.51
1:D:357:THR:HG21	1:D:505:MET:HB3	1.91	0.51
1:A:120:ASP:HA	1:A:123:LYS:HE2	1.92	0.51
1:B:162:ARG:HD2	1:B:163:LYS:HE2	1.94	0.50
1:A:289:ASP:HB2	6:A:2049:HOH:O	2.12	0.49
1:C:84:THR:HA	1:C:310:GLN:HG3	1.95	0.49
1:D:429:PRO:HG2	1:D:431:PHE:CE2	2.48	0.49
1:B:162:ARG:HD3	2:B:600:APX:H2A	1.95	0.48
1:A:262:TYR:CE1	6:A:2310:HOH:O	2.55	0.48
1:B:260:ARG:HH21	1:B:580:SER:HB3	1.79	0.48
1:D:412:ILE:O	1:D:416:VAL:HG23	2.14	0.47
1:C:180:ASN:ND2	6:C:2095:HOH:O	2.46	0.47
1:A:506:HIS:HD2	6:A:2357:HOH:O	1.95	0.47
1:B:226:HIS:CD2	1:B:228:PHE:HB2	2.49	0.47
1:D:260:ARG:HD3	1:D:587:PHE:CE2	2.51	0.46
1:D:584:ASP:HA	1:D:594:GLN:O	2.15	0.46
1:C:275:SER:O	1:C:303:THR:HA	2.16	0.46
1:D:172:ARG:HA	1:D:176:PHE:O	2.15	0.46
1:D:84:THR:O	1:D:485:SER:HB3	2.16	0.46
1:D:116:PRO:O	1:D:119:PRO:HD2	2.16	0.45
1:C:529:ALA:HB3	1:C:530:PRO:HD3	1.97	0.45
1:D:496:GLU:OE2	5:D:620:DMV:O31	2.35	0.45
1:A:506:HIS:CD2	6:A:2357:HOH:O	2.67	0.44
1:B:123:LYS:HE2	1:B:286:ARG:HG2	1.99	0.44
1:C:224:LEU:O	1:C:248:ALA:HA	2.18	0.44
1:D:145:LYS:HB3	1:D:145:LYS:HE2	1.81	0.43
1:B:96:GLU:OE1	1:B:109:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:O	1:B:248:ALA:HA	2.18	0.43
1:D:337:ARG:HD2	1:D:541:LEU:HD13	2.00	0.43
1:D:165:SER:N	6:D:2073:HOH:O	2.50	0.43
1:B:370:LEU:HA	1:B:370:LEU:HD23	1.88	0.43
1:D:313:LYS:HD3	6:D:2255:HOH:O	2.19	0.43
1:A:589:ARG:HG3	6:A:2551:HOH:O	2.19	0.43
1:B:443:LYS:HA	1:B:443:LYS:HD3	1.79	0.43
1:B:123:LYS:HD3	6:B:2039:HOH:O	2.19	0.42
1:B:529:ALA:HB3	1:B:530:PRO:HD3	1.99	0.42
1:A:84:THR:O	1:A:485:SER:HB3	2.20	0.42
1:B:242:LYS:HA	1:B:242:LYS:HD3	1.85	0.42
1:C:530:PRO:HG3	1:D:534:TYR:CG	2.55	0.42
1:B:496:GLU:OE2	5:B:620:DMV:O31	2.38	0.42
1:D:380:GLY:O	1:D:462:PRO:HB3	2.20	0.42
1:A:330:ILE:HD11	1:A:471:LEU:HD13	2.02	0.42
1:D:224:LEU:O	1:D:248:ALA:HA	2.20	0.42
1:D:561:ASP:HA	1:D:562:PRO:HD2	1.92	0.42
1:A:553:ASP:HB2	6:A:2600:HOH:O	2.19	0.41
1:B:242:LYS:NZ	1:B:281:GLN:OE1	2.50	0.41
1:C:221:ILE:HG12	1:C:245:SER:HB2	2.02	0.41
1:A:261:LEU:O	1:A:271:ALA:HB3	2.21	0.41
1:A:574:ARG:HA	1:A:575:PRO:HD3	1.92	0.41
1:B:275:SER:O	1:B:303:THR:HA	2.21	0.41
1:A:318:GLY:HA3	1:A:492:GLU:OE2	2.21	0.41
1:A:518:SER:O	1:A:522:ARG:HG3	2.20	0.41
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.87	0.41
1:C:345:GLU:OE2	1:C:440:ARG:HD2	2.21	0.41
1:C:508:ARG:NH1	1:C:594:GLN:HB2	2.36	0.40
1:B:276:SER:HB3	1:B:304:PHE:CZ	2.56	0.40
1:D:387:ALA:HB1	1:D:467:VAL:HG23	2.03	0.40
1:D:518:SER:O	1:D:522:ARG:HG3	2.20	0.40
1:B:162:ARG:HD3	2:B:600:APX:C2A	2.50	0.40
1:B:209:TYR:CE1	1:B:210:GLU:HG3	2.57	0.40
1:A:447:LYS:HE2	1:A:447:LYS:CA	2.52	0.40
1:B:372:LEU:HD12	6:B:2297:HOH:O	2.21	0.40
1:C:319:GLU:O	1:C:324:LEU:HB2	2.21	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	516/524 (98%)	499 (97%)	16 (3%)	1 (0%)	51	27
1	B	513/524 (98%)	499 (97%)	13 (2%)	1 (0%)	51	27
1	C	514/524 (98%)	504 (98%)	9 (2%)	1 (0%)	51	27
1	D	511/524 (98%)	492 (96%)	19 (4%)	0	100	100
All	All	2054/2096 (98%)	1994 (97%)	57 (3%)	3 (0%)	55	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	LYS
1	C	163	LYS
1	A	268	VAL

### 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	428/433 (99%)	427 (100%)	1 (0%)	94	90
1	B	426/433 (98%)	423 (99%)	3 (1%)	87	77
1	C	427/433 (99%)	424 (99%)	3 (1%)	87	77
1	D	423/433 (98%)	419 (99%)	4 (1%)	82	69
All	All	1704/1732 (98%)	1693 (99%)	11 (1%)	87	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	TYR
1	B	163	LYS
1	B	312	TYR
1	B	457	LEU
1	C	85	THR
1	C	457	LEU
1	C	553	ASP
1	D	163	LYS
1	D	312	TYR
1	D	346	ASP
1	D	554	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	506	HIS
1	C	180	ASN
1	D	180	ASN
1	D	572	GLN

### 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](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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	APX	A	600	-	33,43,43	1.93	5 (15%)	39,67,67	1.31	3 (7%)
4	SO4	A	603	-	4,4,4	0.76	0	6,6,6	0.39	0
5	DMV	A	620	3	5,9,9	4.72	2 (40%)	3,13,13	1.19	0
2	APX	B	600	-	33,43,43	1.92	5 (15%)	39,67,67	1.29	3 (7%)
5	DMV	B	620	3	5,9,9	4.87	2 (40%)	3,13,13	1.15	0
2	APX	C	600	-	33,43,43	1.87	5 (15%)	39,67,67	1.26	2 (5%)
5	DMV	C	620	3	5,9,9	4.58	2 (40%)	3,13,13	1.08	0
2	APX	D	600	-	33,43,43	1.90	7 (21%)	39,67,67	1.31	4 (10%)
5	DMV	D	620	3	5,9,9	5.14	2 (40%)	3,13,13	1.23	1 (33%)

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	APX	A	600	-	1/1/12/13	0/23/69/69	0/4/4/4
4	SO4	A	603	-	-	0/0/0/0	0/0/0/0
5	DMV	A	620	3	-	0/9/13/13	0/0/0/0
2	APX	B	600	-	1/1/12/13	0/23/69/69	0/4/4/4
5	DMV	B	620	3	-	0/9/13/13	0/0/0/0
2	APX	C	600	-	1/1/12/13	0/23/69/69	0/4/4/4
5	DMV	C	620	3	-	0/9/13/13	0/0/0/0
2	APX	D	600	-	1/1/12/13	0/23/69/69	0/4/4/4
5	DMV	D	620	3	-	0/9/13/13	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	620	DMV	O21-C2	-10.69	1.24	1.42
5	B	620	DMV	O21-C2	-10.10	1.25	1.42
5	A	620	DMV	O21-C2	-9.86	1.25	1.42
5	C	620	DMV	O21-C2	-9.56	1.26	1.42
2	D	600	APX	C2A-N3A	-7.46	1.34	1.45
2	C	600	APX	C2A-N3A	-7.44	1.34	1.45
2	B	600	APX	C2A-N3A	-7.41	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	APX	C2A-N3A	-7.30	1.35	1.45
2	A	600	APX	P2-O2B	-5.21	1.50	1.59
2	D	600	APX	P2-O2B	-4.66	1.51	1.59
2	C	600	APX	P2-O2B	-4.42	1.51	1.59
2	B	600	APX	P2-O2B	-4.39	1.51	1.59
2	B	600	APX	P2-OP2	-3.17	1.41	1.54
2	C	600	APX	C5A-C6A	-3.16	1.42	1.51
2	A	600	APX	P2-OP2	-3.12	1.42	1.54
2	B	600	APX	C5A-C6A	-3.08	1.42	1.51
2	D	600	APX	P2-OP2	-3.05	1.42	1.54
2	D	600	APX	C5A-C6A	-2.92	1.42	1.51
2	C	600	APX	P2-OP2	-2.77	1.43	1.54
2	A	600	APX	C5A-C6A	-2.70	1.43	1.51
2	B	600	APX	P2-OP3	-2.64	1.44	1.54
2	A	600	APX	P2-OP3	-2.52	1.44	1.54
2	C	600	APX	P2-OP3	-2.46	1.44	1.54
2	D	600	APX	P2-OP3	-2.39	1.45	1.54
2	D	600	APX	P2-OP1	-2.01	1.43	1.50
2	D	600	APX	O4B-C1B	2.13	1.44	1.41
5	C	620	DMV	C4-C3	2.90	1.58	1.52
5	A	620	DMV	C4-C3	3.28	1.58	1.52
5	B	620	DMV	C4-C3	3.36	1.59	1.52
5	D	620	DMV	C4-C3	3.74	1.59	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	APX	C4B-O4B-C1B	-2.62	106.98	109.77
2	D	600	APX	C4B-O4B-C1B	-2.40	107.21	109.77
2	A	600	APX	C2A-N3A-C4A	-2.27	119.20	122.19
2	C	600	APX	C2A-N3A-C4A	-2.23	119.25	122.19
2	B	600	APX	C2A-N3A-C4A	-2.14	119.38	122.19
2	D	600	APX	C2A-N3A-C4A	-2.12	119.40	122.19
5	D	620	DMV	O31-C3-C32	-2.05	103.73	108.48
2	D	600	APX	O1N-C1M-O4M	-2.00	108.45	111.14
2	B	600	APX	O4M-C1M-C2M	2.55	107.68	104.46
2	A	600	APX	N1A-C2A-N3A	5.16	122.07	111.83
2	C	600	APX	N1A-C2A-N3A	5.26	122.28	111.83
2	B	600	APX	N1A-C2A-N3A	5.30	122.35	111.83
2	D	600	APX	N1A-C2A-N3A	5.45	122.65	111.83

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	600	APX	C6A
2	A	600	APX	C6A
2	D	600	APX	C6A
2	C	600	APX	C6A

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	APX	1	0
4	A	603	SO4	1	0
2	B	600	APX	2	0
5	B	620	DMV	1	0
5	D	620	DMV	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	514/524 (98%)	-0.44	6 (1%) 79 80	4, 8, 20, 53	0
1	B	510/524 (97%)	-0.25	9 (1%) 69 69	5, 12, 28, 53	0
1	C	512/524 (97%)	-0.02	15 (2%) 52 51	9, 15, 31, 60	0
1	D	513/524 (97%)	0.25	23 (4%) 34 32	10, 19, 33, 48	0
All	All	2049/2096 (97%)	-0.11	53 (2%) 56 55	4, 14, 31, 60	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	595	ALA	11.4
1	C	595	ALA	10.1
1	C	85	THR	10.0
1	C	84	THR	8.0
1	D	164	GLY	7.2
1	A	82	SER	5.6
1	D	595	ALA	4.9
1	D	83	ALA	4.7
1	C	163	LYS	4.1
1	B	594	GLN	4.0
1	C	164	GLY	3.9
1	B	163	LYS	3.5
1	D	166	ASN	3.4
1	C	106	TYR	3.3
1	A	84	THR	3.2
1	D	85	THR	3.2
1	D	163	LYS	3.2
1	D	179	GLU	3.1
1	C	87	ASP	3.1
1	A	85	THR	3.0
1	D	154	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	447	LYS	2.9
1	B	154	ASP	2.9
1	A	576	SER	2.9
1	B	164	GLY	2.9
1	B	179	GLU	2.9
1	D	180	ASN	2.8
1	D	103	HIS	2.8
1	D	188	GLU	2.7
1	A	83	ALA	2.5
1	D	84	THR	2.5
1	D	423	TYR	2.5
1	C	593	ARG	2.5
1	D	342	GLY	2.5
1	B	106	TYR	2.4
1	D	576	SER	2.4
1	C	154	ASP	2.4
1	C	423	TYR	2.3
1	D	444	VAL	2.3
1	D	594	GLN	2.3
1	D	347	LEU	2.3
1	C	102	GLY	2.3
1	D	340	GLU	2.2
1	D	577	VAL	2.2
1	D	211	LYS	2.2
1	C	89	ASP	2.2
1	B	87	ASP	2.2
1	C	173	ALA	2.2
1	C	86	PHE	2.1
1	A	423	TYR	2.1
1	B	91	SER	2.1
1	C	166	ASN	2.1
1	D	165	SER	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
4	SO4	A	603	5/5	0.96	0.17	8.89	22,23,24,24	0
5	DMV	D	620	10/10	0.85	0.14	3.55	15,16,17,18	0
5	DMV	B	620	10/10	0.92	0.11	3.43	8,9,9,11	0
5	DMV	A	620	10/10	0.94	0.11	2.69	4,6,6,7	0
2	APX	A	600	40/40	0.95	0.10	1.67	9,17,27,29	0
5	DMV	C	620	10/10	0.94	0.10	1.59	10,11,12,12	0
2	APX	B	600	40/40	0.97	0.08	-0.28	10,15,19,20	0
2	APX	C	600	40/40	0.97	0.07	-0.39	12,17,21,21	0
2	APX	D	600	40/40	0.95	0.09	-0.43	17,20,25,26	0
3	MN	B	602	1/1	1.00	0.06	-1.31	11,11,11,11	0
3	MN	A	602	1/1	0.99	0.04	-2.28	7,7,7,7	0
3	MN	C	602	1/1	0.99	0.04	-2.41	12,12,12,12	0
3	MN	D	602	1/1	0.99	0.04	-4.85	15,15,15,15	0
3	MN	B	601	1/1	0.99	0.04	-	8,8,8,8	0
3	MN	C	601	1/1	0.99	0.04	-	10,10,10,10	0
3	MN	D	601	1/1	0.97	0.05	-	14,14,14,14	0
3	MN	A	601	1/1	1.00	0.04	-	6,6,6,6	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.