



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MNQ  
Title : Crystal structure of myosin-2 motor domain in complex with ADP-metavanadate and resveratrol  
Authors : Schneider, J.; Taft, M.; Backhaus, A.; Baruch, P.; Fedorov, R.; Manstein, D.J.  
Deposited on : 2010-04-22  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

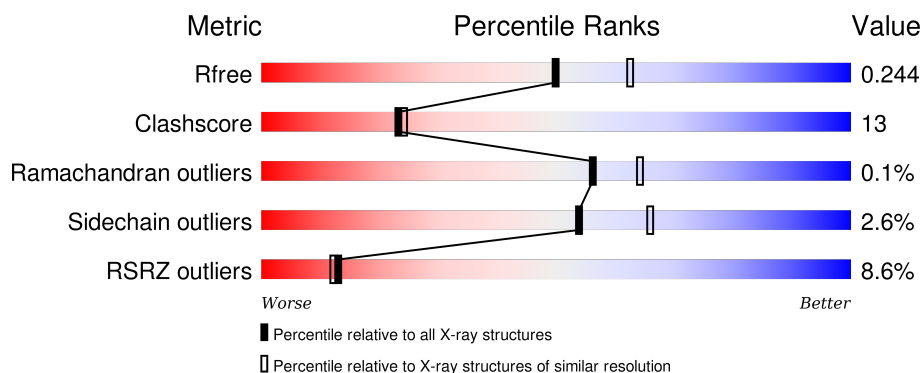
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	788	<div> <div>8%</div> <div>72%</div> <div>20%</div> <div>7%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	STL	A	902	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	780	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6819 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 Myosin-2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	735	5943	3769	1027	1130	17	0	5	0

There are 28 discrepancies between the modelled and reference sequences:

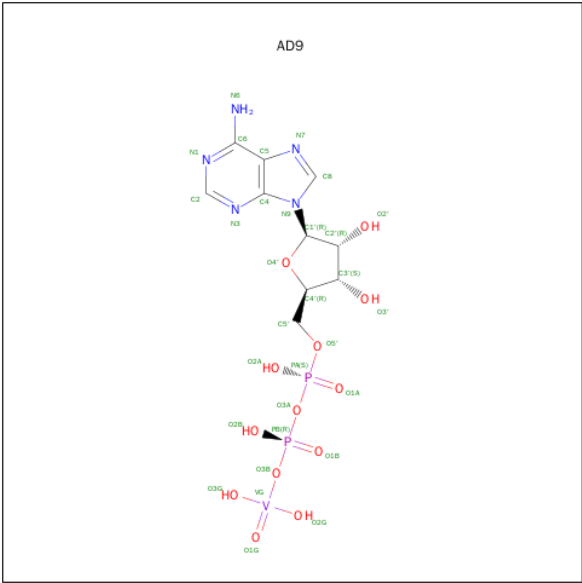
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P08799
A	-9	HIS	-	EXPRESSION TAG	UNP P08799
A	-8	HIS	-	EXPRESSION TAG	UNP P08799
A	-7	HIS	-	EXPRESSION TAG	UNP P08799
A	-6	HIS	-	EXPRESSION TAG	UNP P08799
A	-5	HIS	-	EXPRESSION TAG	UNP P08799
A	-4	HIS	-	EXPRESSION TAG	UNP P08799
A	-3	HIS	-	EXPRESSION TAG	UNP P08799
A	-2	ASP	-	EXPRESSION TAG	UNP P08799
A	-1	GLY	-	EXPRESSION TAG	UNP P08799
A	0	THR	-	EXPRESSION TAG	UNP P08799
A	1	GLU	-	EXPRESSION TAG	UNP P08799
A	2	ASP	-	EXPRESSION TAG	UNP P08799
A	762	LEU	-	EXPRESSION TAG	UNP P08799
A	763	GLU	-	EXPRESSION TAG	UNP P08799
A	764	SER	-	EXPRESSION TAG	UNP P08799
A	765	ASN	-	EXPRESSION TAG	UNP P08799
A	766	GLU	-	EXPRESSION TAG	UNP P08799
A	767	PRO	-	EXPRESSION TAG	UNP P08799
A	768	PRO	-	EXPRESSION TAG	UNP P08799
A	769	MET	-	EXPRESSION TAG	UNP P08799
A	770	ASP	-	EXPRESSION TAG	UNP P08799
A	771	PHE	-	EXPRESSION TAG	UNP P08799
A	772	ASP	-	EXPRESSION TAG	UNP P08799
A	773	ASP	-	EXPRESSION TAG	UNP P08799
A	774	ASP	-	EXPRESSION TAG	UNP P08799
A	776	PRO	-	EXPRESSION TAG	UNP P08799

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Chain	Residue	Modelled	Actual	Comment	Reference
A	777	PHE	-	EXPRESSION TAG	UNP P08799

- Molecule 2 is ADP METAVANADATE (three-letter code: AD9) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>2</sub>V).

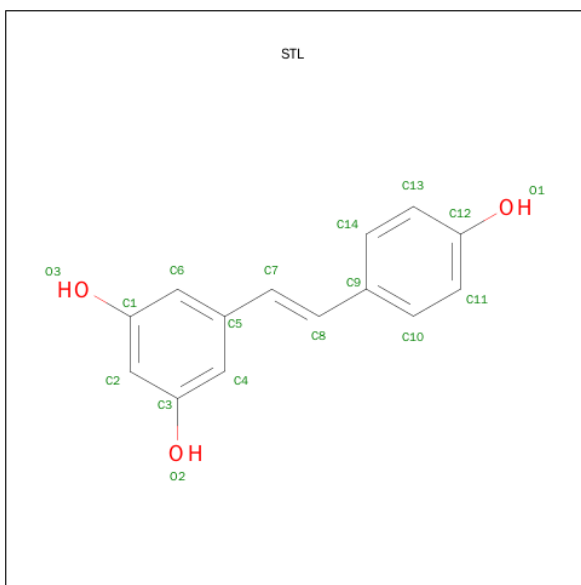


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	V		
2	A	1	31	10	5	13	2	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is RESVERATROL (three-letter code: STL) (formula: C<sub>14</sub>H<sub>12</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	14	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

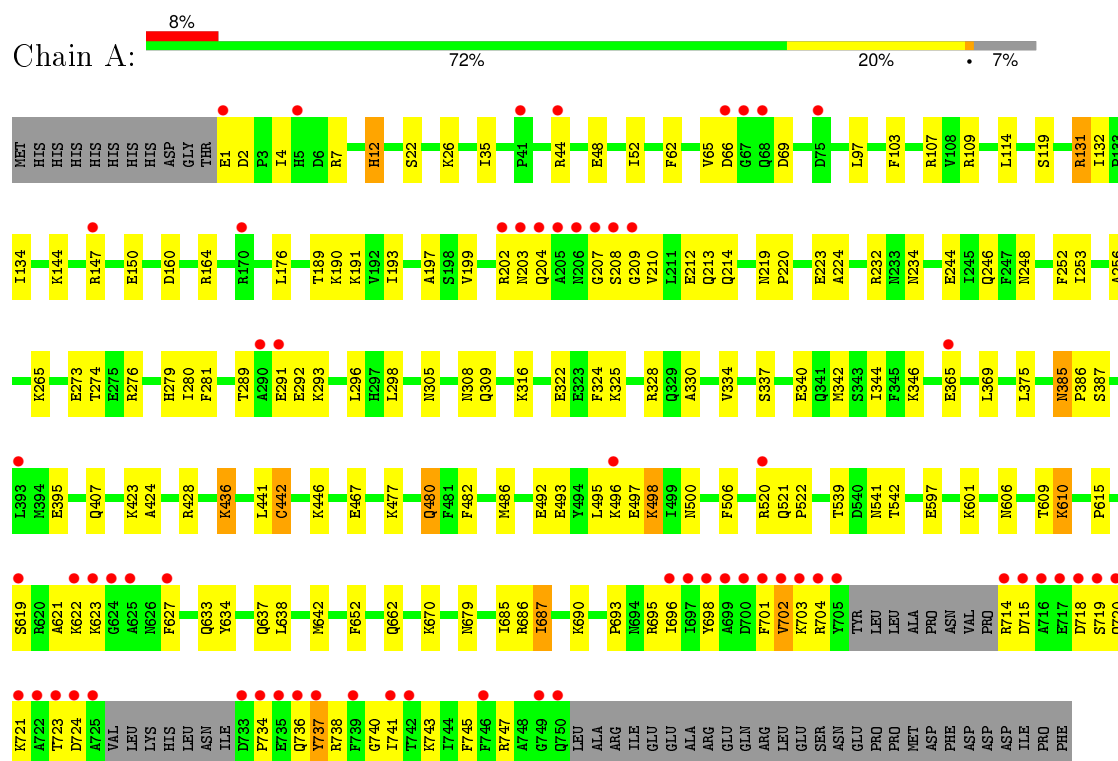
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	811	Total	O	0	0
			811	811		

### 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: Myosin-2 heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.90Å 147.90Å 153.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.64 – 2.20 19.64 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.64-2.20) 99.7 (19.64-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.88 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.201 , 0.250 0.200 , 0.244	Depositor DCC
$R_{free}$ test set	2560 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.6	EDS
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51199 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.375 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: STL, MG, EDO, AD9

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	0.34	0/6058	0.56	0/8168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	5943	0	5874	157	0
2	A	31	0	14	2	0
3	A	1	0	0	0	0
4	A	17	0	9	3	0
5	A	16	0	24	1	0
6	A	811	0	0	23	0
All	All	6819	0	5921	160	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 13.

All (160) 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:202:ARG:HB3	1:A:208:SER:HB3	1.37	1.06
1:A:442[A]:CYS:O	1:A:442[A]:CYS:SG	2.36	0.82
1:A:698:TYR:HD1	1:A:719:SER:HG	1.27	0.81
1:A:480:GLN:HE21	1:A:480:GLN:HA	1.46	0.81
1:A:704:ARG:O	1:A:704:ARG:HD2	1.82	0.80
1:A:291:GLU:HG3	6:A:1339:HOH:O	1.83	0.78
1:A:190:LYS:HE2	1:A:219:ASN:HD21	1.49	0.77
1:A:695:ARG:HD3	1:A:745:PHE:CE2	2.20	0.76
1:A:436:LYS:HA	1:A:436:LYS:NZ	2.01	0.76
1:A:97:LEU:HD23	1:A:686:ARG:HG2	1.68	0.74
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.69	0.73
1:A:721:LYS:C	1:A:723:THR:H	1.91	0.72
1:A:234:ASN:HD21	4:A:902:STL:H10	1.54	0.72
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.91	0.70
1:A:219:ASN:HB3	1:A:220:PRO:HD3	1.74	0.70
1:A:477:LYS:HD3	1:A:638:LEU:HD21	1.74	0.70
1:A:610:LYS:HD3	6:A:1808:HOH:O	1.93	0.69
1:A:492:GLU:O	1:A:496:LYS:HG2	1.96	0.66
1:A:248:ASN:HD21	1:A:252:PHE:HB2	1.63	0.64
1:A:493:GLU:HG2	1:A:695:ARG:NE	2.13	0.64
1:A:436:LYS:HA	1:A:436:LYS:HZ2	1.63	0.62
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.81	0.62
1:A:385:ASN:ND2	1:A:387:SER:H	1.97	0.62
1:A:385:ASN:HD22	1:A:385:ASN:C	2.04	0.61
1:A:273:GLU:HG2	1:A:274:THR:HG23	1.83	0.61
1:A:736:GLN:HB3	6:A:1789:HOH:O	2.00	0.61
1:A:718:ASP:C	1:A:720:GLN:N	2.54	0.60
1:A:520:ARG:HD2	6:A:1338:HOH:O	2.01	0.60
1:A:322:GLU:HG3	6:A:1744:HOH:O	2.03	0.58
1:A:615:PRO:O	1:A:619:SER:HB2	2.02	0.58
2:A:900:AD9:O1G	2:A:900:AD9:VG	1.58	0.58
1:A:467:GLU:HG3	5:A:780:EDO:H12	1.86	0.57
1:A:633:GLN:O	1:A:637:GLN:HG3	2.04	0.57
1:A:202:ARG:CB	1:A:208:SER:HB3	2.24	0.56
1:A:369:LEU:HD23	1:A:375:LEU:HD22	1.88	0.56
1:A:385:ASN:HD22	1:A:386:PRO:N	2.04	0.56
1:A:714:ARG:HH21	1:A:714:ARG:HG2	1.71	0.56
1:A:365:GLU:H	1:A:365:GLU:CD	2.09	0.55
1:A:144:LYS:HG3	1:A:199:VAL:HG23	1.87	0.55
1:A:103:PHE:HE2	1:A:107:ARG:NH2	2.05	0.55
1:A:256:ALA:HB3	1:A:441[A]:LEU:HD13	1.88	0.55
1:A:687:ILE:O	1:A:687:ILE:HD13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLU:OE1	1:A:65:VAL:HG21	2.08	0.54
1:A:234:ASN:H	1:A:662:GLN:HE22	1.55	0.54
1:A:610:LYS:NZ	1:A:610:LYS:HB2	2.22	0.54
1:A:498:LYS:HZ2	1:A:498:LYS:HB3	1.71	0.54
1:A:721:LYS:C	1:A:723:THR:N	2.61	0.54
1:A:324:PHE:O	1:A:328:ARG:HG3	2.08	0.54
1:A:634:TYR:HA	1:A:637:GLN:HE21	1.72	0.53
1:A:539:THR:OG1	1:A:542:THR:HG23	2.08	0.53
1:A:482:PHE:CZ	1:A:486:MET:HG3	2.43	0.53
1:A:506:PHE:HA	6:A:1319:HOH:O	2.08	0.53
1:A:35:ILE:HD11	1:A:62:PHE:CD2	2.43	0.53
1:A:498:LYS:HG3	1:A:741:ILE:HD11	1.90	0.53
1:A:204:GLN:HB2	1:A:208:SER:OG	2.09	0.52
1:A:541[B]:ASN:ND2	6:A:1708:HOH:O	2.42	0.52
1:A:436:LYS:HE3	6:A:1554:HOH:O	2.08	0.52
1:A:495:LEU:HA	6:A:1566:HOH:O	2.09	0.52
1:A:209:GLY:O	1:A:213:GLN:HB2	2.09	0.52
1:A:131:ARG:HH11	1:A:131:ARG:HG2	1.74	0.52
1:A:498:LYS:HE2	6:A:1566:HOH:O	2.10	0.52
1:A:210:VAL:O	1:A:214:GLN:HG3	2.10	0.52
1:A:2:ASP:OD1	1:A:4:ILE:HG12	2.08	0.52
1:A:204:GLN:NE2	1:A:208:SER:OG	2.42	0.52
1:A:131:ARG:HG2	1:A:131:ARG:NH1	2.25	0.52
1:A:189:THR:O	1:A:193:ILE:HG12	2.10	0.52
1:A:698:TYR:HD1	1:A:719:SER:OG	1.92	0.51
1:A:190:LYS:HE2	1:A:219:ASN:ND2	2.21	0.51
1:A:693:PRO:HD2	1:A:747:ARG:O	2.11	0.51
1:A:606:ASN:O	1:A:609:THR:HG22	2.10	0.51
1:A:293:LYS:HG2	1:A:298:LEU:HD12	1.92	0.51
1:A:248:ASN:ND2	1:A:252:PHE:HB2	2.24	0.51
1:A:160:ASP:O	1:A:164:ARG:HG2	2.11	0.50
1:A:734:PRO:HA	1:A:737:TYR:CE1	2.45	0.50
1:A:520:ARG:CZ	1:A:520:ARG:HB3	2.41	0.50
1:A:702:VAL:HG11	1:A:715:ASP:OD1	2.12	0.50
1:A:207:GLY:HA2	1:A:210:VAL:HG23	1.94	0.50
1:A:395:GLU:HA	1:A:407:GLN:O	2.11	0.49
1:A:477:LYS:HD3	1:A:638:LEU:CD2	2.41	0.49
1:A:204:GLN:HB2	1:A:208:SER:CB	2.41	0.49
1:A:330:ALA:O	1:A:334:VAL:HG23	2.12	0.49
1:A:212:GLU:H	1:A:212:GLU:CD	2.15	0.49
1:A:497:GLU:O	1:A:740:GLY:HA2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG23	1:A:52:ILE:HD11	1.94	0.49
1:A:202:ARG:HB3	1:A:208:SER:CB	2.27	0.49
1:A:342:MET:HG2	6:A:1696:HOH:O	2.11	0.49
1:A:265:LYS:HE2	1:A:423:LYS:HB3	1.95	0.49
1:A:714:ARG:HG2	1:A:715:ASP:H	1.77	0.49
1:A:714:ARG:HG2	1:A:715:ASP:N	2.28	0.49
1:A:495:LEU:HD23	1:A:495:LEU:C	2.33	0.48
1:A:736:GLN:HA	1:A:747:ARG:HB2	1.94	0.48
1:A:701:PHE:O	1:A:701:PHE:CG	2.66	0.48
1:A:436:LYS:HA	1:A:436:LYS:HZ3	1.75	0.48
1:A:718:ASP:C	1:A:720:GLN:H	2.15	0.48
1:A:316:LYS:HB3	6:A:1772:HOH:O	2.14	0.47
1:A:244:GLU:O	1:A:256:ALA:HA	2.14	0.47
1:A:337:SER:OG	1:A:340:GLU:HG3	2.14	0.47
1:A:622:LYS:O	1:A:622:LYS:HG2	2.15	0.47
1:A:35:ILE:C	1:A:35:ILE:HD12	2.35	0.46
1:A:385:ASN:HD22	1:A:386:PRO:CD	2.28	0.46
1:A:696:ILE:HD12	1:A:696:ILE:N	2.31	0.46
1:A:690:LYS:HE3	6:A:1316:HOH:O	2.15	0.46
1:A:308:ASN:OD1	1:A:309:GLN:NE2	2.45	0.46
1:A:686:ARG:HD2	6:A:1575:HOH:O	2.15	0.46
1:A:97:LEU:HD23	1:A:686:ARG:CG	2.42	0.46
1:A:103:PHE:CE2	1:A:107:ARG:NH2	2.83	0.45
1:A:497:GLU:HB3	1:A:740:GLY:HA3	1.97	0.45
1:A:638:LEU:O	1:A:642:MET:HG2	2.16	0.45
1:A:197:ALA:HA	1:A:253:ILE:CD1	2.46	0.45
1:A:190:LYS:HE2	1:A:223:GLU:OE1	2.17	0.45
1:A:342:MET:O	1:A:346:LYS:HG3	2.17	0.45
1:A:385:ASN:ND2	1:A:385:ASN:C	2.69	0.45
1:A:621:ALA:HB1	1:A:623:LYS:HG3	1.98	0.45
1:A:718:ASP:CB	1:A:720:GLN:HB2	2.47	0.44
1:A:718:ASP:HB3	1:A:720:GLN:HB2	1.98	0.44
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.99	0.44
1:A:7:ARG:HH21	1:A:7:ARG:HG3	1.83	0.44
1:A:670:LYS:HB3	6:A:1334:HOH:O	2.18	0.44
1:A:737:TYR:O	1:A:738:ARG:HD3	2.17	0.44
2:A:900:AD9:H4'	6:A:1315:HOH:O	2.16	0.44
1:A:35:ILE:HD12	1:A:35:ILE:O	2.16	0.44
1:A:147:ARG:HB2	1:A:150:GLU:HG3	2.00	0.43
1:A:424:ALA:O	1:A:428:ARG:HG3	2.18	0.43
1:A:500:ASN:HB3	6:A:1569:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLN:HA	1:A:522:PRO:HA	1.94	0.43
1:A:316:LYS:HD2	6:A:1112:HOH:O	2.19	0.42
1:A:246:GLN:HB3	1:A:446:LYS:HB3	2.01	0.42
1:A:493:GLU:HG2	1:A:695:ARG:HE	1.83	0.42
1:A:22:SER:O	1:A:26:LYS:HG3	2.19	0.42
1:A:132:ILE:HG22	1:A:134:ILE:HG23	2.02	0.42
1:A:202:ARG:HB3	1:A:208:SER:O	2.20	0.42
1:A:276:ARG:HH21	1:A:279:HIS:HD1	1.68	0.42
1:A:203:ASN:HD22	1:A:203:ASN:N	2.18	0.42
1:A:325:LYS:HE3	6:A:1798:HOH:O	2.20	0.42
1:A:234:ASN:HD21	4:A:902:STL:C10	2.29	0.42
1:A:7:ARG:HA	1:A:12:HIS:CG	2.55	0.42
1:A:497:GLU:HG3	1:A:745:PHE:CZ	2.55	0.41
1:A:702:VAL:HG12	1:A:702:VAL:O	2.19	0.41
1:A:704:ARG:O	1:A:704:ARG:CD	2.61	0.41
1:A:597:GLU:O	1:A:601:LYS:HG3	2.21	0.41
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.85	0.41
1:A:289:THR:O	1:A:293:LYS:HG3	2.19	0.41
1:A:203:ASN:ND2	1:A:203:ASN:N	2.69	0.41
1:A:246:GLN:HB3	1:A:446:LYS:CB	2.51	0.41
1:A:224:ALA:HB2	6:A:1483:HOH:O	2.20	0.41
1:A:745:PHE:N	1:A:745:PHE:CD1	2.89	0.41
1:A:305:ASN:ND2	6:A:1740:HOH:O	2.53	0.41
1:A:740:GLY:N	1:A:743:LYS:O	2.49	0.41
1:A:305:ASN:O	1:A:309:GLN:HG2	2.21	0.41
1:A:197:ALA:HA	1:A:253:ILE:HD12	2.03	0.41
1:A:340:GLU:O	1:A:344:ILE:HG13	2.20	0.41
1:A:232:ARG:NH1	6:A:1324:HOH:O	2.53	0.41
1:A:176:LEU:HD12	1:A:652:PHE:CE1	2.56	0.41
1:A:273:GLU:C	1:A:274:THR:HG23	2.41	0.40
1:A:498:LYS:HA	1:A:498:LYS:HZ3	1.85	0.40
1:A:35:ILE:HD11	1:A:62:PHE:CE2	2.56	0.40
1:A:280:ILE:HG23	1:A:281:PHE:N	2.36	0.40
4:A:902:STL:H11	6:A:1772:HOH:O	2.21	0.40
1:A:622:LYS:HA	1:A:627:PHE:HA	2.04	0.40
1:A:119:SER:OG	1:A:685:ILE:HD11	2.21	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	734/788 (93%)	688 (94%)	45 (6%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	702	VAL

### 5.3.2 Protein sidechains [i](#)

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	647/691 (94%)	629 (97%)	18 (3%)	51	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	12	HIS
1	A	66	ASP
1	A	69	ASP
1	A	131	ARG
1	A	191	LYS
1	A	385	ASN
1	A	436	LYS
1	A	442[A]	CYS
1	A	442[B]	CYS

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	498	LYS
1	A	610	LYS
1	A	679	ASN
1	A	687	ILE
1	A	703	LYS
1	A	724	ASP
1	A	737	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	203	ASN
1	A	204	GLN
1	A	219	ASN
1	A	235	ASN
1	A	305	ASN
1	A	338	GLN
1	A	385	ASN
1	A	480	GLN
1	A	511	GLN
1	A	613	ASN
1	A	637	GLN
1	A	662	GLN
1	A	679	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z  > 2$
5	EDO	A	778	-	3,3,3	0.33	0	2,2,2	0.39	0
5	EDO	A	779	-	3,3,3	0.31	0	2,2,2	0.37	0
5	EDO	A	780	-	3,3,3	0.30	0	2,2,2	0.36	0
2	AD9	A	900	3,6	24,33,33	3.01	8 (33%)	30,52,52	2.10	9 (30%)
4	STL	A	902	-	18,18,18	1.61	4 (22%)	24,24,24	0.58	0
5	EDO	A	903	-	3,3,3	0.32	0	2,2,2	0.36	0

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
5	EDO	A	778	-	-	0/1/1/1	0/0/0/0
5	EDO	A	779	-	-	0/1/1/1	0/0/0/0
5	EDO	A	780	-	-	0/1/1/1	0/0/0/0
2	AD9	A	900	3,6	-	0/12/38/38	0/3/3/3
4	STL	A	902	-	-	0/5/5/5	0/2/2/2
5	EDO	A	903	-	-	0/1/1/1	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	STL	C9-C8	2.05	1.53	1.47
4	A	902	STL	C4-C3	2.14	1.42	1.39
4	A	902	STL	C2-C3	2.20	1.42	1.39
2	A	900	AD9	PA-O1A	2.28	1.54	1.48
4	A	902	STL	C2-C1	2.29	1.42	1.39
2	A	900	AD9	PB-O3A	2.67	1.65	1.60
2	A	900	AD9	C2-N3	2.69	1.36	1.32
2	A	900	AD9	PB-O2B	2.98	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	AD9	PA-O3A	3.09	1.66	1.60
2	A	900	AD9	O4'-C1'	4.28	1.46	1.41
2	A	900	AD9	PB-O1B	8.09	1.69	1.48
2	A	900	AD9	PA-O2A	9.12	1.70	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	AD9	O3B-PB-O1B	-4.21	98.71	108.80
2	A	900	AD9	O3A-PB-O1B	-4.11	98.94	108.79
2	A	900	AD9	N3-C2-N1	-3.50	126.22	128.89
2	A	900	AD9	O2A-PA-O3A	-2.52	101.92	108.79
2	A	900	AD9	O5'-PA-O1A	2.14	117.55	108.56
2	A	900	AD9	PA-O5'-C5'	2.24	127.96	120.25
2	A	900	AD9	O3A-PA-O1A	2.69	115.24	108.79
2	A	900	AD9	O2B-PB-O3B	3.01	116.95	108.80
2	A	900	AD9	O3B-PB-O3A	6.13	112.64	100.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	780	EDO	1	0
2	A	900	AD9	2	0
4	A	902	STL	3	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	735/788 (93%)	0.32	63 (8%) <b>13</b> <b>12</b>	21, 39, 65, 73	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	705	TYR	9.1
1	A	205	ALA	8.2
1	A	206	ASN	8.1
1	A	207	GLY	7.7
1	A	716	ALA	6.9
1	A	699	ALA	6.9
1	A	208	SER	6.8
1	A	734	PRO	6.7
1	A	720	GLN	6.7
1	A	717	GLU	6.4
1	A	746	PHE	6.4
1	A	721	LYS	6.3
1	A	741	ILE	6.1
1	A	700	ASP	6.0
1	A	701	PHE	5.9
1	A	725	ALA	5.9
1	A	203	ASN	5.8
1	A	737	TYR	5.7
1	A	704	ARG	5.6
1	A	698	TYR	5.2
1	A	715	ASP	5.2
1	A	696	ILE	5.1
1	A	722	ALA	5.1
1	A	723	THR	5.0
1	A	714	ARG	5.0
1	A	724	ASP	4.7
1	A	702	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	204	GLN	4.4
1	A	209	GLY	4.2
1	A	718	ASP	4.1
1	A	697	ILE	3.8
1	A	291	GLU	3.6
1	A	1	GLU	3.6
1	A	622	LYS	3.6
1	A	749	GLY	3.4
1	A	67	GLY	3.4
1	A	202	ARG	3.4
1	A	623	LYS	3.3
1	A	625	ALA	3.2
1	A	703	LYS	3.2
1	A	735	GLU	3.1
1	A	147	ARG	3.0
1	A	496	LYS	3.0
1	A	66	ASP	3.0
1	A	170	ARG	2.9
1	A	750	GLN	2.8
1	A	624	GLY	2.7
1	A	75	ASP	2.7
1	A	733	ASP	2.7
1	A	719	SER	2.7
1	A	393	LEU	2.6
1	A	365	GLU	2.6
1	A	41	PRO	2.6
1	A	5	HIS	2.6
1	A	736	GLN	2.5
1	A	44	ARG	2.4
1	A	68	GLN	2.4
1	A	742	THR	2.3
1	A	520	ARG	2.3
1	A	619	SER	2.1
1	A	627	PHE	2.1
1	A	739	PHE	2.1
1	A	290	ALA	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	STL	A	902	17/17	0.71	0.47	12.91	64,64,65,65	0
5	EDO	A	780	4/4	0.86	0.30	12.37	68,69,69,69	0
5	EDO	A	903	4/4	0.84	0.24	0.79	66,67,67,67	0
3	MG	A	901	1/1	0.98	0.15	0.14	29,29,29,29	0
2	AD9	A	900	31/31	0.97	0.13	-0.20	26,29,32,42	0
5	EDO	A	778	4/4	0.98	0.08	-0.77	30,32,33,33	0
5	EDO	A	779	4/4	0.73	0.56	-	62,62,63,64	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.