



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:07 pm BST

PDB ID : 3MYL  
Title : Insights into the Importance of Hydrogen Bonding in the Gamma-Phosphate Binding Pocket of Myosin: Structural and Functional Studies of Ser236  
Authors : Frye, J.J.; Klenchin, V.A.; Bagshaw, C.R.; Rayment, I.  
Deposited on : 2010-05-10  
Resolution : 2.00 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.

---

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

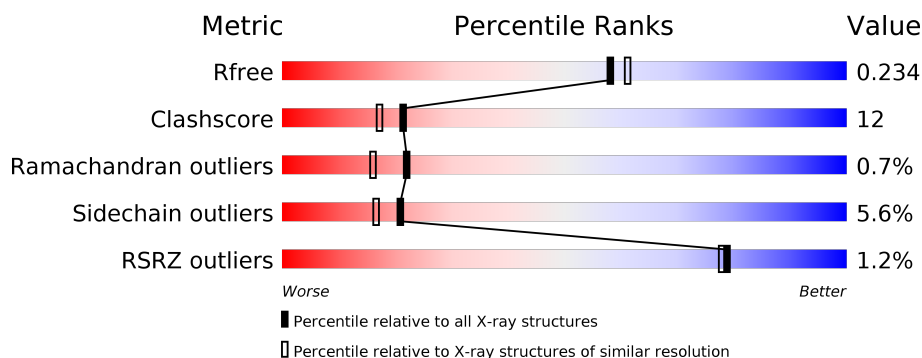
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	X	762	<div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6715 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
1	X	744	Total	C	N	O	S	0	8	0
			5969	3801	1019	1133	16			

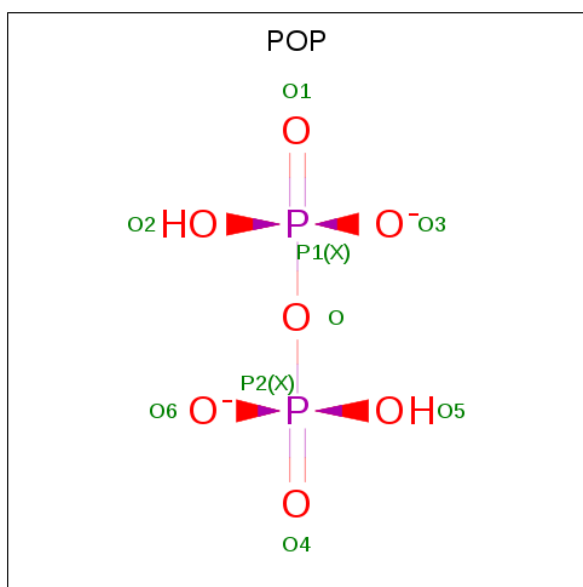
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	GLY	-	EXPRESSION TAG	UNP P08799
X	236	ALA	SER	ENGINEERED MUTATION	UNP P08799
X	760	LEU	-	EXPRESSION TAG	UNP P08799
X	761	PRO	-	EXPRESSION TAG	UNP P08799
X	762	ASN	-	EXPRESSION TAG	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	O	P	0	0
			9	7	2		

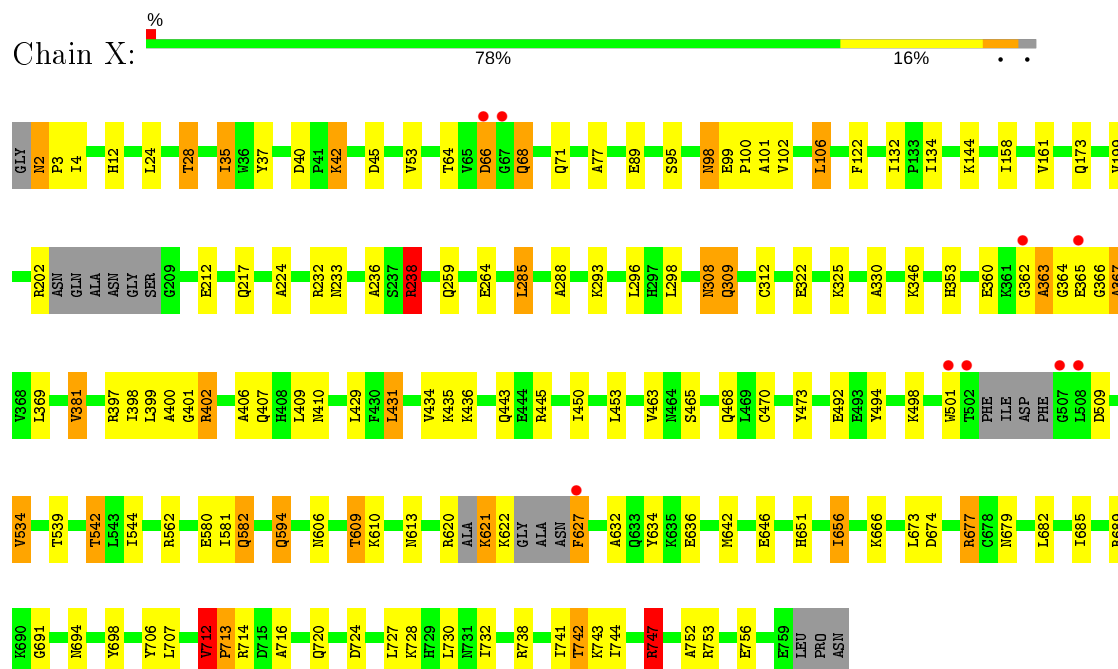
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	736	Total	O	0	0
			736	736		

### 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: Myosin-2 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.05 Å   180.78 Å   53.89 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.69 – 2.00 29.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.69-2.00) 98.7 (29.69-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.185   ,   0.244 0.178   ,   0.234	Depositor DCC
$R_{free}$ test set	3483 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POP

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	X	1.19	12/6105 (0.2%)	1.00	17/8247 (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	X	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	636	GLU	CG-CD	10.53	1.67	1.51
1	X	636	GLU	CB-CG	6.93	1.65	1.52
1	X	636	GLU	CD-OE1	6.54	1.32	1.25
1	X	473	TYR	CD1-CE1	6.15	1.48	1.39
1	X	473	TYR	CD2-CE2	5.92	1.48	1.39
1	X	238	ARG	CD-NE	-5.75	1.36	1.46
1	X	434	VAL	CB-CG2	5.58	1.64	1.52
1	X	224	ALA	CA-CB	5.39	1.63	1.52
1	X	161	VAL	CB-CG2	5.39	1.64	1.52
1	X	122	PHE	CE2-CZ	5.08	1.47	1.37
1	X	632	ALA	CA-CB	5.07	1.63	1.52
1	X	89	GLU	CB-CG	5.01	1.61	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	238	ARG	NE-CZ-NH2	-12.61	113.99	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	238	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	X	753	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	X	712	VAL	C-N-CD	-9.49	99.73	120.60
1	X	747	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	X	677	ARG	NE-CZ-NH1	-9.28	115.66	120.30
1	X	689	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	X	431	LEU	CA-CB-CG	8.11	133.96	115.30
1	X	689	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	X	738	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	X	753	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	X	636	GLU	OE1-CD-OE2	-5.52	116.67	123.30
1	X	453	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	X	106	LEU	CA-CB-CG	5.34	127.59	115.30
1	X	402	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	X	738	ARG	CG-CD-NE	-5.12	101.04	111.80
1	X	620	ARG	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	712	VAL	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	X	5969	0	5855	142	0
2	X	1	0	0	0	0
3	X	9	0	0	0	0
4	X	736	0	0	25	0
All	All	6715	0	5855	142	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 12.

All (142) 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:X:35:ILE:HD11	1:X:77:ALA:HB1	1.25	1.17
1:X:747:ARG:HH11	1:X:747:ARG:HG3	1.05	1.12
1:X:443:GLN:HB3	4:X:1724:HOH:O	1.49	1.10
1:X:40:ASP:OD2	1:X:42:LYS:HG2	1.55	1.06
1:X:742:THR:HG21	4:X:1532:HOH:O	1.62	0.99
1:X:539:THR:H	1:X:542:THR:CG2	1.81	0.93
1:X:622:LYS:C	1:X:627:PHE:CE2	2.43	0.91
1:X:747:ARG:HH11	1:X:747:ARG:CG	1.76	0.91
1:X:465:SER:H	1:X:468:GLN:HE21	1.20	0.88
1:X:691:GLY:O	1:X:747:ARG:HD3	1.72	0.88
1:X:609:THR:HG23	4:X:1248:HOH:O	1.74	0.86
1:X:747:ARG:HG3	1:X:747:ARG:NH1	1.90	0.85
1:X:582:GLN:H	1:X:582:GLN:HE21	1.22	0.82
1:X:742:THR:HG22	1:X:743:LYS:HG3	1.61	0.80
1:X:35:ILE:CD1	1:X:77:ALA:HB1	2.07	0.80
1:X:363:ALA:O	1:X:365:GLU:N	2.14	0.78
1:X:360:GLU:O	1:X:367:ALA:HA	1.85	0.77
1:X:144:LYS:HE2	1:X:199:VAL:HG12	1.64	0.77
1:X:2[B]:ASN:HB3	1:X:3:PRO:HD3	1.67	0.77
1:X:706:TYR:HE1	1:X:714:ARG:HH11	1.31	0.76
1:X:322[B]:GLU:OE2	1:X:325:LYS:NZ	2.20	0.74
1:X:2[A]:ASN:C	1:X:2[A]:ASN:HD22	1.91	0.74
1:X:492:GLU:OE1	4:X:1633:HOH:O	2.05	0.74
1:X:494:TYR:CE1	1:X:501:TRP:HB3	2.23	0.73
1:X:443:GLN:CB	4:X:1724:HOH:O	2.18	0.72
1:X:498:LYS:HE2	1:X:741:ILE:HD11	1.72	0.72
1:X:622:LYS:HA	1:X:627:PHE:CD2	2.26	0.71
1:X:232:ARG:HD3	4:X:1507:HOH:O	1.90	0.71
1:X:582:GLN:N	1:X:582:GLN:HE21	1.90	0.69
1:X:293:LYS:HD2	1:X:298:LEU:HB2	1.75	0.69
1:X:362:GLY:O	1:X:363:ALA:HB2	1.92	0.69
1:X:308:ASN:C	1:X:308:ASN:HD22	1.93	0.68
1:X:45:ASP:HB2	1:X:673:LEU:HD13	1.75	0.68
1:X:674[A]:ASP:CG	4:X:1790:HOH:O	2.34	0.66
1:X:707:LEU:HB2	4:X:1312:HOH:O	1.97	0.64
1:X:296:LEU:O	1:X:353:HIS:HE1	1.81	0.64
1:X:362:GLY:O	1:X:363:ALA:CB	2.46	0.63
1:X:238:ARG:HD3	1:X:264:GLU:OE1	1.99	0.63
1:X:217:GLN:HE21	1:X:330:ALA:HA	1.63	0.63
1:X:609:THR:CG2	4:X:1248:HOH:O	2.40	0.62
1:X:12:HIS:ND1	4:X:1487:HOH:O	2.31	0.62
1:X:285:LEU:O	1:X:293:LYS:HE2	1.99	0.62

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:144:LYS:CE	1:X:199:VAL:HG12	2.29	0.62
1:X:399:LEU:HD11	1:X:401:GLY:O	1.98	0.61
1:X:656:ILE:HD11	1:X:679:ASN:ND2	2.15	0.61
1:X:353:HIS:HD2	4:X:1733:HOH:O	1.83	0.61
1:X:202:ARG:N	1:X:212:GLU:OE2	2.30	0.60
1:X:365:GLU:HG2	1:X:410:ASN:HA	1.83	0.59
1:X:594:GLN:HE21	1:X:594:GLN:HA	1.68	0.59
1:X:40:ASP:CG	1:X:42:LYS:HG2	2.22	0.59
1:X:747:ARG:NH1	1:X:747:ARG:CG	2.51	0.59
1:X:698:TYR:CE1	1:X:720:GLN:HG2	2.38	0.58
1:X:28:THR:CG2	4:X:1395:HOH:O	2.51	0.58
1:X:308:ASN:HD21	1:X:309[B]:GLN:NE2	2.02	0.58
1:X:642:MET:O	1:X:646:GLU:CG	2.52	0.57
1:X:465:SER:H	1:X:468:GLN:NE2	1.97	0.57
1:X:68:GLN:HG2	4:X:1525:HOH:O	2.04	0.57
1:X:346:LYS:O	1:X:381:VAL:CG1	2.53	0.56
1:X:627:PHE:N	4:X:1723:HOH:O	2.38	0.56
1:X:539:THR:H	1:X:542:THR:HG23	1.69	0.56
1:X:713:PRO:HB2	1:X:716:ALA:HB2	1.89	0.55
1:X:463:VAL:HG12	4:X:1742:HOH:O	2.05	0.55
1:X:366:GLY:O	1:X:409:LEU:O	2.24	0.55
1:X:609:THR:HG22	1:X:613:ASN:OD1	2.07	0.55
1:X:724:ASP:O	1:X:728:LYS:HG2	2.07	0.54
1:X:95:SER:HA	1:X:694:ASN:HD21	1.72	0.54
1:X:656:ILE:HD11	1:X:679:ASN:HD21	1.73	0.54
1:X:399:LEU:HD13	1:X:399:LEU:C	2.28	0.54
1:X:712:VAL:N	1:X:713:PRO:HD2	2.22	0.53
1:X:238:ARG:CD	1:X:264:GLU:OE1	2.57	0.53
1:X:308:ASN:ND2	1:X:308:ASN:C	2.62	0.53
1:X:45:ASP:HB2	1:X:673:LEU:CD1	2.37	0.53
1:X:621:LYS:HD3	1:X:622:LYS:H	1.74	0.53
1:X:2[A]:ASN:ND2	1:X:4:ILE:H	2.07	0.52
1:X:642:MET:O	1:X:646:GLU:HG3	2.09	0.52
1:X:28:THR:HG22	4:X:1395:HOH:O	2.08	0.51
1:X:677:ARG:HD3	4:X:1515:HOH:O	2.10	0.51
1:X:621:LYS:HD3	1:X:622:LYS:N	2.25	0.51
1:X:173:GLN:HB2	1:X:450:ILE:HG12	1.93	0.51
1:X:539:THR:H	1:X:542:THR:HG22	1.73	0.51
1:X:2[A]:ASN:HD22	1:X:3:PRO:N	2.09	0.51
1:X:366:GLY:O	1:X:367:ALA:HB3	2.10	0.50
1:X:443:GLN:HG3	1:X:445:ARG:H	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:580:GLU:O	1:X:580:GLU:HG3	2.11	0.50
1:X:68:GLN:O	1:X:68:GLN:HG3	2.10	0.50
1:X:399:LEU:HD13	1:X:400:ALA:N	2.27	0.49
1:X:706:TYR:CD1	1:X:714:ARG:HG3	2.48	0.49
1:X:642:MET:O	1:X:646:GLU:HG2	2.11	0.49
1:X:677:ARG:CG	1:X:682:LEU:HD12	2.43	0.48
1:X:621:LYS:CD	1:X:622:LYS:H	2.26	0.47
1:X:296:LEU:HB2	1:X:298:LEU:HG	1.96	0.47
1:X:312:CYS:HB2	4:X:1827:HOH:O	2.15	0.47
1:X:706:TYR:HE1	1:X:714:ARG:NH1	2.06	0.47
1:X:677:ARG:HG2	1:X:682:LEU:HD12	1.96	0.47
1:X:398:ILE:HD12	1:X:407:GLN:HG3	1.97	0.46
1:X:28:THR:HG23	4:X:1395:HOH:O	2.14	0.46
1:X:98:ASN:ND2	1:X:100:PRO:HG2	2.31	0.46
1:X:397:ARG:HA	1:X:406:ALA:HA	1.97	0.46
1:X:64:THR:HG23	1:X:68:GLN:O	2.16	0.46
1:X:562[A]:ARG:HD3	4:X:1648:HOH:O	2.15	0.46
1:X:293:LYS:HD3	1:X:298:LEU:HD12	1.97	0.45
1:X:66:ASP:OD1	1:X:66:ASP:N	2.47	0.45
1:X:727:LEU:HD22	1:X:732:ILE:HD13	1.98	0.45
1:X:4:ILE:HG22	1:X:4:ILE:O	2.16	0.45
1:X:365:GLU:HG2	1:X:410:ASN:CA	2.47	0.45
1:X:622:LYS:C	1:X:627:PHE:CZ	2.90	0.45
1:X:132:ILE:HG22	1:X:134:ILE:HG23	1.98	0.45
1:X:37:TYR:OH	1:X:64:THR:HB	2.17	0.45
1:X:581:ILE:HD12	1:X:581:ILE:C	2.36	0.45
1:X:233:ASN:HB3	1:X:236:ALA:HB2	1.99	0.45
1:X:544:ILE:HB	1:X:581:ILE:HG12	1.98	0.45
1:X:102:VAL:HG21	1:X:685:ILE:HD13	1.99	0.44
1:X:288:ALA:HB3	1:X:293:LYS:HD3	2.00	0.44
1:X:435:LYS:HG2	4:X:1719:HOH:O	2.17	0.44
1:X:398:ILE:HD12	1:X:407:GLN:CG	2.48	0.43
1:X:99:GLU:OE2	4:X:1429:HOH:O	2.21	0.43
1:X:674[A]:ASP:OD1	4:X:1790:HOH:O	2.21	0.43
1:X:2[A]:ASN:HD22	1:X:4:ILE:H	1.65	0.43
1:X:666:LYS:HE3	1:X:666:LYS:HB3	1.42	0.43
1:X:232:ARG:CD	4:X:1507:HOH:O	2.59	0.43
1:X:534:VAL:HG13	1:X:534:VAL:O	2.17	0.43
1:X:98:ASN:ND2	1:X:101:ALA:H	2.17	0.42
1:X:293:LYS:HA	1:X:298:LEU:HD12	2.02	0.42
1:X:346:LYS:O	1:X:381:VAL:HG13	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:622:LYS:CA	1:X:627:PHE:CD2	3.00	0.42
1:X:40:ASP:OD2	1:X:40:ASP:C	2.57	0.42
1:X:2[A]:ASN:C	1:X:2[A]:ASN:ND2	2.64	0.42
1:X:365:GLU:HA	1:X:366:GLY:HA3	1.50	0.42
1:X:158:ILE:HD11	1:X:651:HIS:HB3	2.00	0.42
1:X:539:THR:OG1	1:X:542:THR:HG22	2.20	0.42
1:X:694:ASN:ND2	4:X:1152:HOH:O	2.52	0.42
1:X:470:CYS:HB3	1:X:634:TYR:CZ	2.55	0.41
1:X:706:TYR:CE1	1:X:714:ARG:HG3	2.55	0.41
1:X:2[B]:ASN:CB	1:X:3:PRO:HD3	2.39	0.41
1:X:582:GLN:H	1:X:582:GLN:NE2	2.04	0.41
1:X:621:LYS:HD3	1:X:621:LYS:HA	1.36	0.41
1:X:95:SER:HB3	1:X:752:ALA:HB2	2.02	0.41
1:X:752:ALA:O	1:X:756:GLU:HG3	2.21	0.41
1:X:365:GLU:HG2	1:X:410:ASN:HB2	2.03	0.40
1:X:606:ASN:O	1:X:610:LYS:HD3	2.21	0.40
1:X:698:TYR:CZ	1:X:720:GLN:HG2	2.56	0.40
1:X:366:GLY:O	1:X:367:ALA:CB	2.68	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	X	743/762 (98%)	725 (98%)	13 (2%)	5 (1%)	22 16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	363	ALA
1	X	364	GLY
1	X	713	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	X	509	ASP
1	X	367	ALA

### 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	X	637/664 (96%)	600 (94%)	37 (6%)	20	15

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	2[A]	ASN
1	X	2[B]	ASN
1	X	24	LEU
1	X	28	THR
1	X	35	ILE
1	X	42	LYS
1	X	53	VAL
1	X	66	ASP
1	X	68	GLN
1	X	71	GLN
1	X	98	ASN
1	X	106	LEU
1	X	238	ARG
1	X	259	GLN
1	X	285	LEU
1	X	308	ASN
1	X	309[A]	GLN
1	X	309[B]	GLN
1	X	369	LEU
1	X	381	VAL
1	X	402	ARG
1	X	429	LEU
1	X	431	LEU
1	X	436	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	X	534	VAL
1	X	542	THR
1	X	582	GLN
1	X	594	GLN
1	X	609	THR
1	X	621	LYS
1	X	627	PHE
1	X	656	ILE
1	X	712	VAL
1	X	730	LEU
1	X	742	THR
1	X	744	ILE
1	X	747	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	38	ASN
1	X	71	GLN
1	X	98	ASN
1	X	194	GLN
1	X	213	GLN
1	X	217	GLN
1	X	234	ASN
1	X	283	GLN
1	X	305	ASN
1	X	308	ASN
1	X	329	GLN
1	X	353	HIS
1	X	439	ASN
1	X	468	GLN
1	X	479	GLN
1	X	483	ASN
1	X	491	GLN
1	X	521	GLN
1	X	582	GLN
1	X	594	GLN
1	X	694	ASN
1	X	720	GLN
1	X	729	HIS

### 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
3	POP	X	999	2	6,8,8	1.02	1 (16%)	13,13,13	0.71	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
3	POP	X	999	2	-	1/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	999	POP	P1-O2	-2.15	1.46	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	999	POP	P2-O-P1-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	X	744/762 (97%)	-0.27	9 (1%) 79 78	7, 20, 40, 59	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	508	LEU	4.8
1	X	501	TRP	4.7
1	X	365	GLU	4.6
1	X	627	PHE	3.3
1	X	507	GLY	3.2
1	X	362	GLY	3.0
1	X	66	ASP	2.5
1	X	67	GLY	2.2
1	X	502	THR	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	MG	X	998	1/1	0.99	0.10	10,10,10,10	0
3	POP	X	999	9/9	0.99	0.08	7,8,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.