



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:18 am GMT

PDB ID : 4E7S  
Title : Myosin VI D23R I24R R569E (MD) pre-powerstroke state  
Authors : Isabet, T.; Sweeney, H.L.; Houdusse, A.  
Deposited on : 2012-03-19  
Resolution : 2.25 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

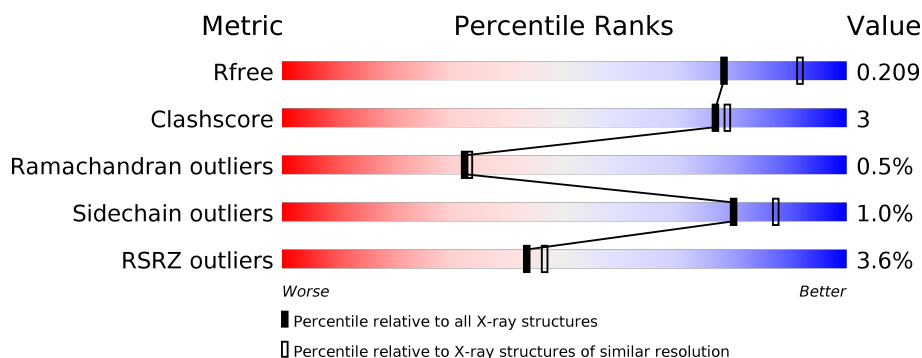
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	798	
1	B	798	

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
5	GOL	A	804	-	-	-	X
5	GOL	A	805	-	-	-	X
5	GOL	A	806	-	-	-	X
5	GOL	B	806	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12540 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-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	2	0
			6034	3843	1040	1122	29			
1	B	752	Total	C	N	O	S	0	1	0
			5930	3781	1023	1098	28			

There are 26 discrepancies between the modelled and reference sequences:

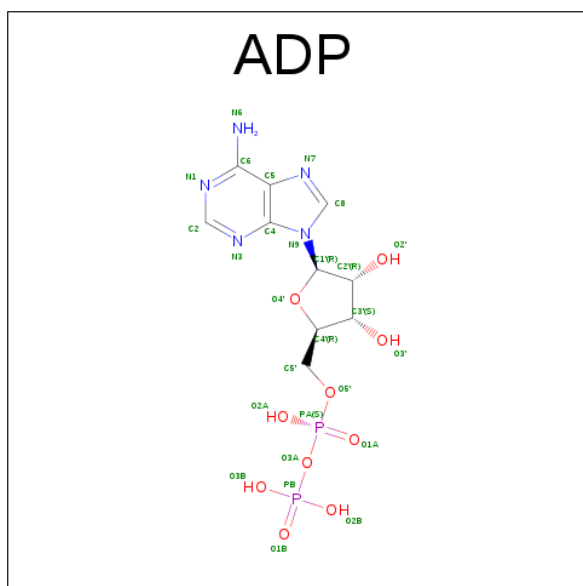
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP F1RQI7
A	-7	ASP	-	EXPRESSION TAG	UNP F1RQI7
A	-6	TYR	-	EXPRESSION TAG	UNP F1RQI7
A	-5	LYS	-	EXPRESSION TAG	UNP F1RQI7
A	-4	ASP	-	EXPRESSION TAG	UNP F1RQI7
A	-3	ASP	-	EXPRESSION TAG	UNP F1RQI7
A	-2	ASP	-	EXPRESSION TAG	UNP F1RQI7
A	-1	ASP	-	EXPRESSION TAG	UNP F1RQI7
A	0	LYS	-	EXPRESSION TAG	UNP F1RQI7
A	1	GLY	-	EXPRESSION TAG	UNP F1RQI7
A	23	ARG	ASP	ENGINEERED MUTATION	UNP F1RQI7
A	24	ARG	ILE	ENGINEERED MUTATION	UNP F1RQI7
A	569	GLU	ARG	ENGINEERED MUTATION	UNP F1RQI7
B	-8	MET	-	EXPRESSION TAG	UNP F1RQI7
B	-7	ASP	-	EXPRESSION TAG	UNP F1RQI7
B	-6	TYR	-	EXPRESSION TAG	UNP F1RQI7
B	-5	LYS	-	EXPRESSION TAG	UNP F1RQI7
B	-4	ASP	-	EXPRESSION TAG	UNP F1RQI7
B	-3	ASP	-	EXPRESSION TAG	UNP F1RQI7
B	-2	ASP	-	EXPRESSION TAG	UNP F1RQI7
B	-1	ASP	-	EXPRESSION TAG	UNP F1RQI7
B	0	LYS	-	EXPRESSION TAG	UNP F1RQI7
B	1	GLY	-	EXPRESSION TAG	UNP F1RQI7
B	23	ARG	ASP	ENGINEERED MUTATION	UNP F1RQI7
B	24	ARG	ILE	ENGINEERED MUTATION	UNP F1RQI7

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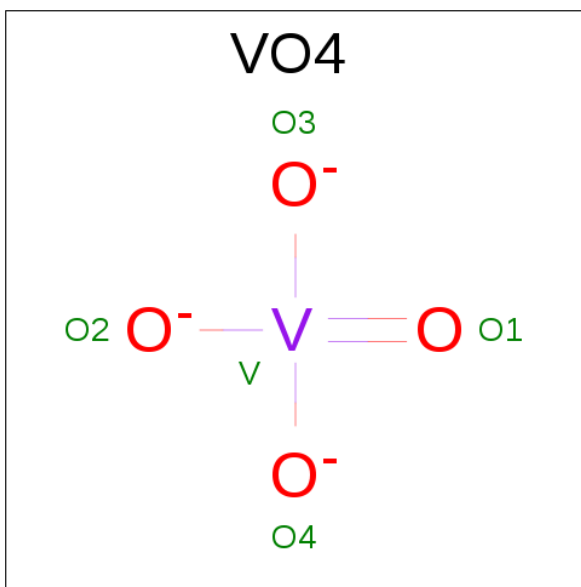
Chain	Residue	Modelled	Actual	Comment	Reference
B	569	GLU	ARG	ENGINEERED MUTATION	UNP F1RQI7

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula:  $O_4V$ ).

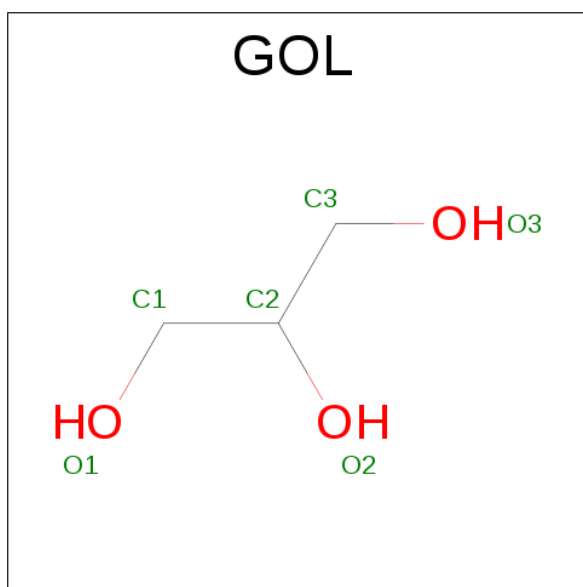


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			5	4	1		
3	B	1	Total	O	V	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

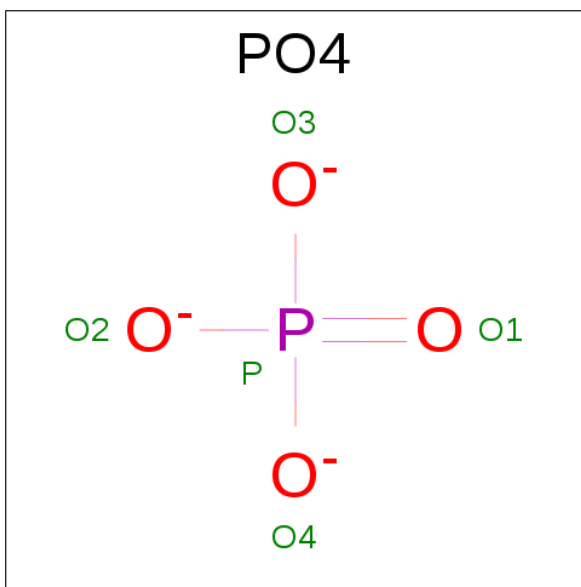
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

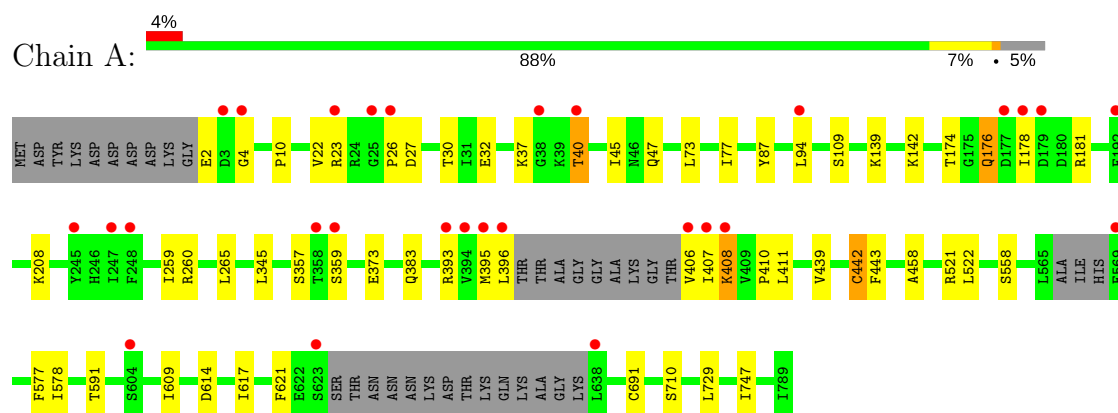
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		
7	B	210	Total	O	0	0
			210	210		



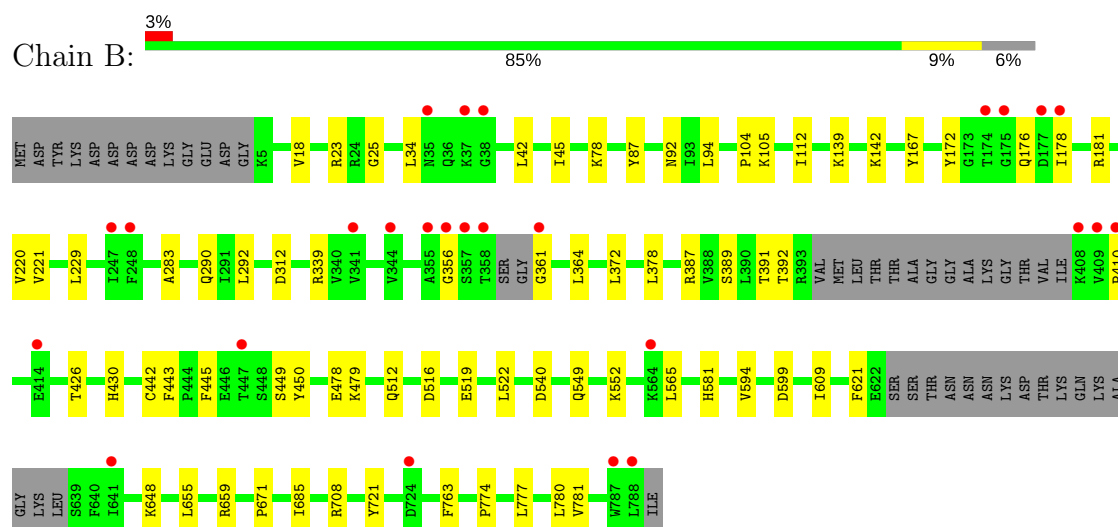
### 3 Residue-property plots [i](#)

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-VI



#### • Molecule 1: Myosin-VI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.95Å 135.14Å 196.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.25 29.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.77-2.25) 98.9 (29.77-2.25)	Depositor EDS
$R_{merge}$	9.20	Depositor
$R_{sym}$	10.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.179 , 0.216 0.169 , 0.209	Depositor DCC
$R_{free}$ test set	5148 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: VO4, GOL, MG, PO4, ADP

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	0.51	0/6158	0.59	0/8315
1	B	0.45	0/6055	0.55	0/8184
All	All	0.48	0/12213	0.57	0/16499

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	6034	0	5865	37	0
1	B	5930	0	5727	44	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	32	3	0
5	B	12	0	16	2	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	259	0	0	6	0
7	B	210	0	0	3	0
All	All	12540	0	11664	82	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 (82) 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:2:GLU:O	1:A:4:GLY:HA2	1.77	0.84
1:A:609:ILE:HG21	1:A:621:PHE:CE1	2.15	0.80
5:A:807:GOL:H31	7:A:1145:HOH:O	1.83	0.78
1:B:292:LEU:HG	5:B:806:GOL:H31	1.66	0.75
1:A:174:THR:HG23	1:A:176:GLN:H	1.56	0.71
1:A:22:VAL:HG23	1:A:23:ARG:H	1.56	0.70
1:B:139:LYS:O	1:B:142:LYS:HE3	1.99	0.62
1:A:10:PRO:HD3	1:A:47:GLN:O	2.02	0.60
1:A:393:ARG:HB2	1:A:411:LEU:HD21	1.85	0.59
1:A:396:LEU:HD12	1:A:406:VAL:N	2.22	0.55
1:B:777:LEU:O	1:B:781:VAL:HG23	2.05	0.55
1:A:609:ILE:HG21	1:A:621:PHE:CD1	2.41	0.55
1:B:387:ARG:O	1:B:391:THR:HG22	2.08	0.54
1:A:591:THR:HG23	7:A:1123:HOH:O	2.06	0.54
1:A:32:GLU:OE1	1:A:40:THR:HG22	2.08	0.54
1:B:18:VAL:HG11	1:B:34:LEU:HD22	1.91	0.53
1:A:208:LYS:HE2	7:A:1060:HOH:O	2.08	0.52
1:A:407:ILE:HG12	1:A:408:LYS:N	2.24	0.52
1:A:521:ARG:O	1:A:522:LEU:HB2	2.10	0.52
1:A:458:ALA:O	7:A:1015:HOH:O	2.19	0.52
1:B:478:GLU:OE1	1:B:581:HIS:HB3	2.10	0.51
1:B:361:GLY:HA2	1:B:410:PRO:HB2	1.94	0.50
1:B:540:ASP:OD1	1:B:594:VAL:HG23	2.11	0.50
1:A:691[B]:CYS:SG	5:A:807:GOL:H11	2.51	0.50
1:B:391:THR:HG23	1:B:392:THR:HG23	1.94	0.50
1:A:729:LEU:HD11	1:B:42:LEU:HB3	1.93	0.49
1:B:479:LYS:HE3	1:B:655:LEU:HD11	1.93	0.49
1:B:142:LYS:HD3	1:B:450:TYR:OH	2.13	0.48
1:B:78:LYS:HD3	7:B:1107:HOH:O	2.12	0.48
1:B:721:TYR:OH	1:B:774:PRO:HB3	2.13	0.48
1:A:396:LEU:O	1:A:396:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ASP:HB3	1:A:617:ILE:HG12	1.96	0.48
1:B:221:VAL:CG1	1:B:445:PHE:HB2	2.44	0.48
1:A:27:ASP:C	1:A:45:ILE:HD12	2.34	0.48
1:A:22:VAL:HG23	1:A:23:ARG:N	2.28	0.47
1:B:512:GLN:NE2	1:B:516:ASP:OD1	2.47	0.47
1:A:395:MET:O	1:A:407:ILE:HG22	2.15	0.47
1:B:25:GLY:O	1:B:45:ILE:HD11	2.14	0.47
1:A:259:ILE:HD12	7:A:990:HOH:O	2.15	0.47
1:B:356:GLY:HA2	1:B:361:GLY:N	2.31	0.46
1:B:339:ARG:HG3	1:B:378:LEU:HD22	1.97	0.46
1:B:565:LEU:HD23	1:B:565:LEU:N	2.31	0.46
1:B:23:ARG:HD3	7:B:1088:HOH:O	2.16	0.46
1:B:478:GLU:OE1	1:B:581:HIS:CB	2.64	0.45
1:A:139:LYS:O	1:A:142:LYS:HD2	2.16	0.45
1:B:522:LEU:HA	1:B:522:LEU:HD23	1.82	0.45
1:B:283:ALA:HA	1:B:312:ASP:OD1	2.17	0.45
1:B:426:THR:HG22	1:B:430:HIS:ND1	2.32	0.45
1:B:655:LEU:HB3	1:B:659:ARG:NH2	2.31	0.45
1:A:27:ASP:O	1:A:45:ILE:HD12	2.17	0.44
1:B:87:TYR:HB3	1:B:94:LEU:HD11	1.99	0.44
5:A:807:GOL:H2	7:A:906:HOH:O	2.16	0.44
1:B:290:GLN:O	5:B:806:GOL:H32	2.18	0.44
1:A:359:SER:O	1:A:410:PRO:HG2	2.18	0.44
1:B:112:ILE:HG23	1:B:167:TYR:CD1	2.53	0.43
1:B:34:LEU:HA	1:B:34:LEU:HD12	1.92	0.43
1:B:609:ILE:HG21	1:B:621:PHE:CZ	2.54	0.43
1:A:10:PRO:CG	1:A:47:GLN:HB3	2.49	0.42
1:A:87:TYR:HB3	1:A:94:LEU:HD11	2.01	0.42
1:B:378:LEU:HA	1:B:378:LEU:HD23	1.89	0.42
1:B:549:GLN:HE22	1:B:552:LYS:HZ1	1.65	0.42
1:A:373:GLU:HG3	1:A:383:GLN:NE2	2.35	0.42
1:A:73:LEU:O	1:A:77:ILE:HG12	2.20	0.42
1:A:178:ILE:HA	1:A:181:ARG:HG3	2.02	0.41
1:B:426:THR:HG22	1:B:430:HIS:CE1	2.55	0.41
1:B:479:LYS:HE3	1:B:655:LEU:CD1	2.50	0.41
1:B:172:TYR:O	1:B:220:VAL:HG23	2.19	0.41
1:B:780:LEU:HA	1:B:780:LEU:HD23	1.83	0.41
1:A:260:ARG:HH21	1:A:260:ARG:HG2	1.85	0.41
1:B:178:ILE:HA	1:B:181:ARG:HB2	2.03	0.41
1:B:104:PRO:O	1:B:105:LYS:HB2	2.20	0.41
1:B:364:LEU:HD22	1:B:372:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:GLU:HB2	1:B:648:LYS:HD2	2.02	0.41
1:B:671:PRO:HA	1:B:685:ILE:HD11	2.03	0.41
1:B:142:LYS:NZ	7:B:972:HOH:O	2.54	0.41
1:A:174:THR:HG23	1:A:176:GLN:N	2.30	0.41
1:A:260:ARG:HG3	1:A:265:LEU:HB2	2.02	0.41
1:B:92:ASN:HB3	1:B:763:PHE:CZ	2.56	0.41
1:A:558:SER:HB2	1:A:578:ILE:HB	2.03	0.41
1:A:22:VAL:HG23	1:A:30:THR:HB	2.02	0.41
1:A:439:VAL:O	1:A:442[B]:CYS:HB2	2.21	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.91	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	756/798 (95%)	734 (97%)	17 (2%)	5 (1%)	25	25
1	B	745/798 (93%)	718 (96%)	25 (3%)	2 (0%)	44	50
All	All	1501/1596 (94%)	1452 (97%)	42 (3%)	7 (0%)	32	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	B	229	LEU
1	B	176	GLN
1	A	40	THR
1	A	176	GLN
1	A	357	SER
1	A	26	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	646/705 (92%)	638 (99%)	8 (1%)	75	84
1	B	628/705 (89%)	622 (99%)	6 (1%)	80	87
All	All	1274/1410 (90%)	1260 (99%)	14 (1%)	80	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	A	408	LYS
1	A	442[A]	CYS
1	A	442[B]	CYS
1	A	443	PHE
1	A	577	PHE
1	A	710	SER
1	A	747	ILE
1	B	389	SER
1	B	442	CYS
1	B	443	PHE
1	B	449	SER
1	B	599	ASP
1	B	708	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	B	549	GLN
1	B	712	HIS

### 5.3.3 RNA

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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	ADP	A	801	3,4	25,29,29	1.06	1 (4%)	24,45,45	1.68	3 (12%)
3	VO4	A	802	2,4	1,4,4	5.09	1 (100%)	0,6,6	0.00	-
5	GOL	A	804	-	5,5,5	0.32	0	5,5,5	0.47	0
5	GOL	A	805	-	5,5,5	0.29	0	5,5,5	0.29	0
5	GOL	A	806	-	5,5,5	0.46	0	5,5,5	0.21	0
5	GOL	A	807	-	5,5,5	0.19	0	5,5,5	0.57	0
2	ADP	B	801	3,4	25,29,29	1.19	2 (8%)	24,45,45	1.75	3 (12%)
3	VO4	B	802	2,4	1,4,4	5.18	1 (100%)	0,6,6	0.00	-
6	PO4	B	804	-	4,4,4	0.81	0	6,6,6	0.39	0
5	GOL	B	805	-	5,5,5	0.28	0	5,5,5	0.56	0
5	GOL	B	806	-	5,5,5	0.27	0	5,5,5	0.26	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
2	ADP	A	801	3,4	-	0/12/32/32	0/3/3/3
3	VO4	A	802	2,4	-	0/0/0/0	0/0/0/0
5	GOL	A	804	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	805	-	-	0/4/4/4	0/0/0/0
5	GOL	A	806	-	-	0/4/4/4	0/0/0/0
5	GOL	A	807	-	-	0/4/4/4	0/0/0/0
2	ADP	B	801	3,4	-	0/12/32/32	0/3/3/3
3	VO4	B	802	2,4	-	0/0/0/0	0/0/0/0
6	PO4	B	804	-	-	0/0/0/0	0/0/0/0
5	GOL	B	805	-	-	0/4/4/4	0/0/0/0
5	GOL	B	806	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ADP	C5-C4	2.67	1.46	1.40
2	A	801	ADP	C5-C4	3.12	1.47	1.40
2	B	801	ADP	PB-O3A	3.15	1.65	1.60
3	A	802	VO4	O1-V	5.09	1.93	1.63
3	B	802	VO4	O1-V	5.18	1.94	1.63

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ADP	N3-C2-N1	-6.37	123.31	128.86
2	A	801	ADP	N3-C2-N1	-5.78	123.83	128.86
2	A	801	ADP	C4-C5-N7	-3.24	106.28	109.41
2	B	801	ADP	C4-C5-N7	-2.92	106.59	109.41
2	B	801	ADP	O2'-C2'-C1'	-2.01	105.33	111.61
2	A	801	ADP	O2A-PA-O1A	2.03	122.81	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	807	GOL	3	0
5	B	806	GOL	2	0

## 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	762/798 (95%)	-0.16	28 (3%)	42 45	32, 47, 73, 115	0
1	B	752/798 (94%)	-0.10	26 (3%)	44 48	36, 52, 82, 124	0
All	All	1514/1596 (94%)	-0.13	54 (3%)	43 46	32, 49, 79, 124	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	LEU	8.8
1	A	359	SER	7.1
1	A	396	LEU	5.9
1	B	358	THR	5.8
1	B	356	GLY	5.3
1	B	355	ALA	5.3
1	A	394	VAL	5.0
1	B	357	SER	4.7
1	B	787	TRP	4.4
1	A	406	VAL	4.3
1	A	358	THR	4.2
1	A	395	MET	4.2
1	A	3	ASP	4.0
1	B	409	VAL	3.9
1	A	407	ILE	3.9
1	B	788	LEU	3.6
1	B	724	ASP	3.3
1	A	178	ILE	3.3
1	A	247	ILE	3.1
1	B	410	PRO	3.0
1	B	361	GLY	2.9
1	B	35	ASN	2.9
1	A	623	SER	2.9
1	B	564	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	344	VAL	2.9
1	A	38	GLY	2.8
1	B	447	THR	2.7
1	A	408	LYS	2.7
1	B	174	THR	2.7
1	B	177	ASP	2.6
1	A	40	THR	2.5
1	A	179	ASP	2.5
1	A	245	TYR	2.5
1	B	37	LYS	2.5
1	A	393	ARG	2.4
1	A	26	PRO	2.4
1	A	23	ARG	2.4
1	A	177	ASP	2.4
1	B	175	GLY	2.4
1	B	641	ILE	2.4
1	A	25	GLY	2.4
1	B	38	GLY	2.4
1	B	408	LYS	2.3
1	B	247	ILE	2.3
1	A	248	PHE	2.3
1	B	414	GLU	2.2
1	A	569	GLU	2.1
1	A	94	LEU	2.1
1	A	192	PHE	2.1
1	B	248	PHE	2.1
1	B	178	ILE	2.0
1	A	604	SER	2.0
1	A	4	GLY	2.0
1	B	341	VAL	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 [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
5	GOL	A	805	6/6	0.85	0.18	6.45	63,65,68,72	0
5	GOL	A	804	6/6	0.95	0.19	5.92	60,63,64,65	0
5	GOL	A	806	6/6	0.71	0.26	5.58	57,61,65,68	0
5	GOL	B	806	6/6	0.94	0.17	2.03	57,62,65,71	0
3	VO4	A	802	5/5	1.00	0.19	0.97	35,35,37,39	0
3	VO4	B	802	5/5	0.99	0.20	0.56	35,35,36,38	0
4	MG	B	803	1/1	0.99	0.20	0.55	35,35,35,35	0
4	MG	A	803	1/1	0.98	0.20	0.40	37,37,37,37	0
2	ADP	A	801	27/27	0.99	0.13	-0.06	30,36,42,43	0
5	GOL	B	805	6/6	0.93	0.12	-0.06	49,53,56,62	0
6	PO4	B	804	5/5	0.97	0.14	-0.19	38,52,58,61	5
2	ADP	B	801	27/27	0.98	0.12	-0.47	30,39,44,44	0
5	GOL	A	807	6/6	0.92	0.12	-0.90	50,51,55,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.