



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:27 PM GMT

PDB ID : 4OZQ  
Title : Crystal structure of the mouse Kif14 motor domain  
Authors : Arora, K.; Talje, L.; Asenjo, A.B.; Andersen, P.; Atchia, K.; Joshi, M.; Sosa, H.; Kwok, B.H.; Allingham, J.S.  
Deposited on : 2014-02-18  
Resolution : 2.71 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

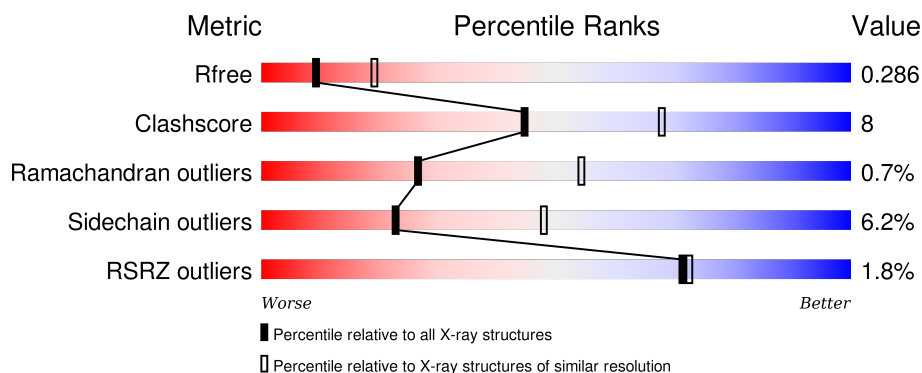
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	720	
1	B	720	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10264 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 Chimera of Maltose-binding periplasmic protein and Kinesin family member 14 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	683	Total	C	N	O	S	0	0	0
			5070	3237	837	980	16			
1	B	687	Total	C	N	O	S	0	0	0
			5096	3253	836	989	18			

There are 20 discrepancies between the modelled and reference sequences:

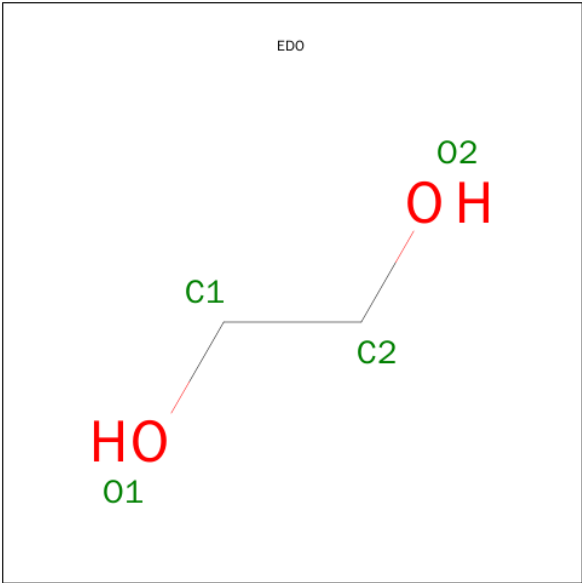
Chain	Residue	Modelled	Actual	Comment	Reference
A	-370	MET	-	expression tag	UNP T9HUW4
A	-8	ALA	-	linker	UNP T9HUW4
A	-7	ALA	-	linker	UNP T9HUW4
A	-6	ALA	-	linker	UNP T9HUW4
A	-5	GLN	-	linker	UNP T9HUW4
A	-4	THR	-	linker	UNP T9HUW4
A	-3	ASN	-	linker	UNP T9HUW4
A	-2	ALA	-	linker	UNP T9HUW4
A	-1	ALA	-	linker	UNP T9HUW4
A	0	ALA	-	linker	UNP T9HUW4
B	-370	MET	-	expression tag	UNP T9HUW4
B	-8	ALA	-	linker	UNP T9HUW4
B	-7	ALA	-	linker	UNP T9HUW4
B	-6	ALA	-	linker	UNP T9HUW4
B	-5	GLN	-	linker	UNP T9HUW4
B	-4	THR	-	linker	UNP T9HUW4
B	-3	ASN	-	linker	UNP T9HUW4
B	-2	ALA	-	linker	UNP T9HUW4
B	-1	ALA	-	linker	UNP T9HUW4
B	0	ALA	-	linker	UNP T9HUW4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 3 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
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

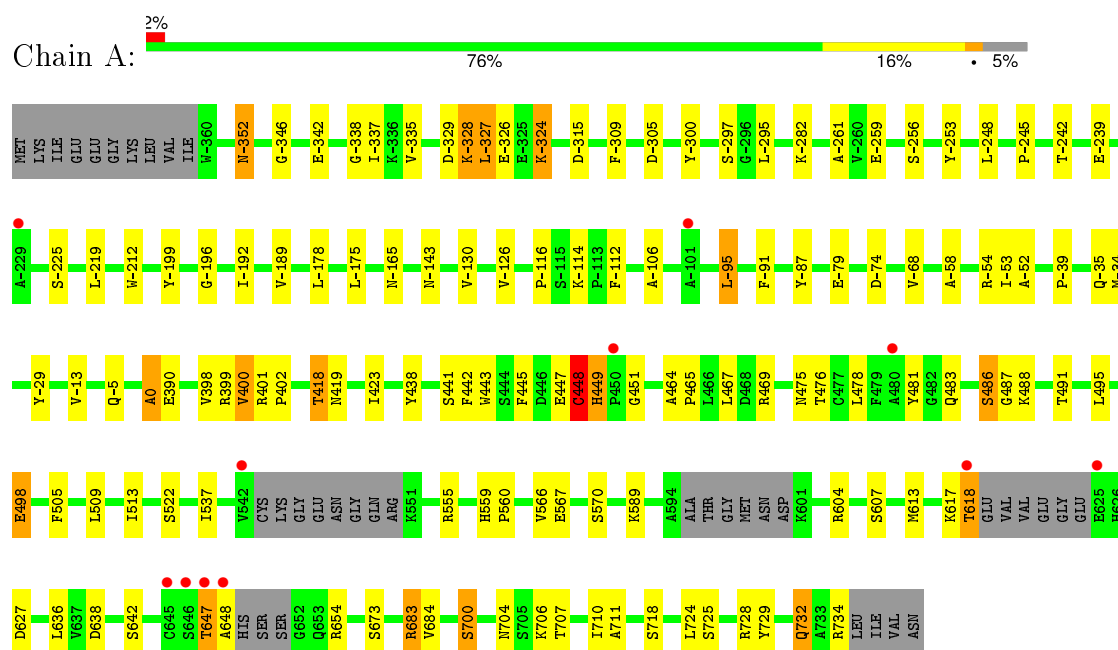
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total 15	O 15	0	0
4	B	21	Total 21	O 21	0	0

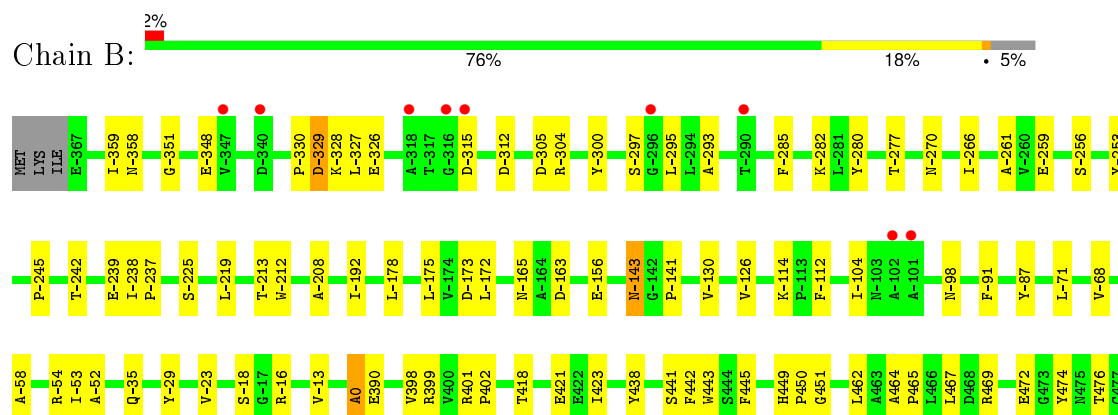
### 3 Residue-property plots [i](#)

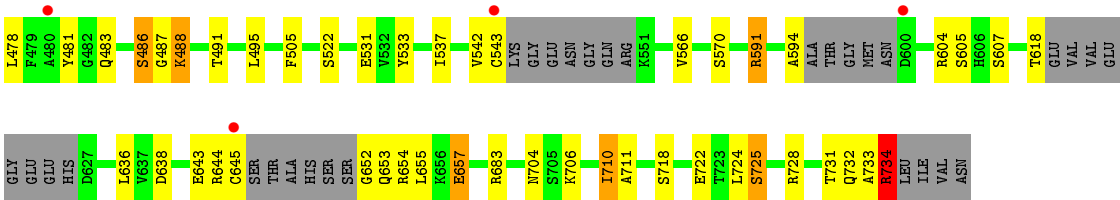
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Chimera of Maltose-binding periplasmic protein and Kinesin family member 14 protein



- Molecule 1: Chimera of Maltose-binding periplasmic protein and Kinesin family member 14 protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.14Å 72.19Å 94.10Å 74.43° 87.45° 89.94°	Depositor
Resolution (Å)	29.36 – 2.71 29.34 – 2.71	Depositor EDS
% Data completeness (in resolution range)	89.5 (29.36-2.71) 83.7 (29.34-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.264 , 0.307 0.245 , 0.286	Depositor DCC
$R_{free}$ test set	2038 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 28.1	EDS
Estimated twinning fraction	0.057 for h,-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 40192 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	0.63	1/5183 (0.0%)	0.73	4/7068 (0.1%)
1	B	0.61	1/5209 (0.0%)	0.74	1/7108 (0.0%)
All	All	0.62	2/10392 (0.0%)	0.74	5/14176 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ALA	C-N	17.10	1.73	1.34
1	B	0	ALA	C-N	14.91	1.68	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	734	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	-305	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	400	VAL	CB-CA-C	5.38	121.63	111.40
1	A	734	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	-305	ASP	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	THR	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	A	5070	0	4777	66	0
1	B	5096	0	4775	90	0
2	A	27	0	12	1	0
2	B	27	0	12	5	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	15	0	0	0	0
4	B	21	0	0	6	0
All	All	10264	0	9588	157	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 8.

All (157) 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:B:0:ALA:C	1:B:390:GLU:N	1.68	1.42
1:A:0:ALA:C	1:A:390:GLU:N	1.73	1.41
1:A:729:TYR:O	1:A:732:GLN:HB2	1.76	0.85
1:B:591:ARG:NH1	1:B:605:SER:O	2.12	0.81
1:B:-329:ASP:O	1:B:-327:LEU:N	2.14	0.78
1:B:594:ALA:HB2	1:B:604:ARG:HD2	1.66	0.77
1:B:418:THR:HG23	1:B:443:TRP:CE3	2.28	0.69
1:B:449:HIS:CD2	1:B:450:PRO:HD2	2.28	0.68
1:B:0:ALA:C	1:B:390:GLU:CA	2.62	0.68
1:B:0:ALA:CA	1:B:390:GLU:N	2.58	0.65
1:B:-178:LEU:HD23	1:B:-13:VAL:HG13	1.80	0.64
1:A:418:THR:HG23	1:A:443:TRP:CE3	2.33	0.64
1:B:449:HIS:HD2	1:B:451:GLY:H	1.45	0.63
1:A:-178:LEU:HD23	1:A:-13:VAL:HG13	1.81	0.63
1:B:-312:ASP:OD2	1:B:-98:ASN:ND2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:GLY:O	1:B:655:LEU:N	2.21	0.62
1:B:604:ARG:HD3	1:B:657:GLU:OE2	1.99	0.62
1:A:617:LYS:O	1:A:627:ASP:HB2	1.99	0.62
1:B:449:HIS:CD2	1:B:451:GLY:H	2.17	0.61
1:B:487:GLY:HA2	2:B:801:ADP:O1A	2.00	0.61
1:B:542:VAL:O	1:B:543:CYS:HB2	2.01	0.61
1:A:-337:ILE:HG21	1:A:-95:LEU:HD21	1.84	0.60
1:B:483:GLN:O	1:B:486:SER:OG	2.19	0.59
1:B:390:GLU:OE2	1:B:474:TYR:OH	2.16	0.59
1:A:-346:GLY:HA3	1:A:-335:VAL:HG21	1.83	0.59
1:A:481:TYR:CZ	1:A:642:SER:OG	2.55	0.59
1:A:483:GLN:O	1:A:486:SER:OG	2.18	0.59
1:B:-29:TYR:CZ	1:B:683:ARG:HG2	2.39	0.58
1:A:487:GLY:HA2	2:A:801:ADP:O1A	2.04	0.57
1:A:513:ILE:HD11	1:A:613:MET:CE	2.35	0.56
1:A:-29:TYR:CZ	1:A:683:ARG:HG2	2.41	0.56
1:B:-285:PHE:O	1:B:-282:LYS:HB2	2.06	0.56
1:A:-326:GLU:N	1:A:-326:GLU:OE1	2.37	0.55
1:A:-199:TYR:CZ	1:A:-196:GLY:HA2	2.42	0.55
1:B:390:GLU:N	1:B:704:ASN:OD1	2.40	0.55
1:B:591:ARG:NH2	1:B:638:ASP:OD2	2.39	0.55
1:B:487:GLY:CA	2:B:801:ADP:O1A	2.55	0.54
1:A:-328:LYS:HG3	1:A:-328:LYS:O	2.07	0.54
1:B:-213:THR:HG21	4:B:907:HOH:O	2.07	0.53
1:B:-23:VAL:HB	4:B:908:HOH:O	2.08	0.53
1:B:643:GLU:N	1:B:643:GLU:OE1	2.26	0.53
1:B:-300:TYR:O	1:B:-295:LEU:HB2	2.09	0.53
1:B:654:ARG:O	1:B:657:GLU:O	2.26	0.53
1:B:-261:ALA:HB2	1:B:-71:LEU:HD22	1.91	0.53
1:A:478:LEU:HB3	1:A:636:LEU:HD23	1.91	0.52
1:A:-39:PRO:HB2	1:A:-34:MET:HG2	1.92	0.52
1:B:478:LEU:HB3	1:B:636:LEU:HD23	1.92	0.52
1:B:449:HIS:CD2	1:B:450:PRO:CD	2.92	0.52
1:B:487:GLY:C	2:B:801:ADP:O1A	2.48	0.52
1:B:733:ALA:O	1:B:734:ARG:HG2	2.09	0.51
1:B:476:THR:HG22	1:B:706:LYS:HB2	1.92	0.51
1:A:-35:GLN:OE1	1:A:-35:GLN:N	2.43	0.51
1:B:-35:GLN:OE1	1:B:-35:GLN:N	2.44	0.51
1:A:498:GLU:HA	1:A:498:GLU:OE2	2.10	0.51
1:B:542:VAL:O	1:B:543:CYS:CB	2.59	0.51
1:B:462:LEU:HD21	1:B:710:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-300:TYR:O	1:A:-295:LEU:HB2	2.11	0.51
1:B:-293:ALA:HB3	1:B:-104:ILE:HG13	1.94	0.49
1:B:-126:VAL:HB	1:B:-54:ARG:HG2	1.94	0.49
1:A:-352:ASN:ND2	1:A:-74:ASP:OD2	2.46	0.49
1:B:465:PRO:O	1:B:469:ARG:HG2	2.12	0.49
1:B:644:ARG:O	1:B:645:CYS:SG	2.71	0.49
1:B:-305:ASP:OD1	1:B:-304:ARG:HG3	2.12	0.49
1:A:617:LYS:O	1:A:627:ASP:CB	2.61	0.48
1:A:481:TYR:O	1:A:711:ALA:HA	2.12	0.48
1:A:465:PRO:O	1:A:469:ARG:HG2	2.13	0.48
1:B:533:TYR:HE1	1:B:657:GLU:OE1	1.97	0.48
1:A:-309:PHE:CE2	1:A:-106:ALA:HB2	2.47	0.48
1:B:-143:ASN:ND2	4:B:906:HOH:O	2.46	0.48
1:B:-326:GLU:N	1:B:-326:GLU:OE1	2.38	0.48
1:A:-126:VAL:HB	1:A:-54:ARG:HG2	1.96	0.47
1:B:481:TYR:O	1:B:711:ALA:HA	2.14	0.47
1:A:0:ALA:CA	1:A:390:GLU:N	2.71	0.47
1:B:469:ARG:NE	1:B:472:GLU:OE2	2.39	0.47
1:B:-156:GLU:OE2	4:B:905:HOH:O	2.20	0.47
1:B:-165:ASN:HB3	1:B:-163:ASP:OD1	2.15	0.46
1:B:533:TYR:CE1	1:B:657:GLU:OE1	2.68	0.46
1:B:418:THR:HG23	1:B:443:TRP:CD2	2.50	0.46
1:B:483:GLN:HA	1:B:643:GLU:OE1	2.16	0.46
1:A:-329:ASP:HB2	1:A:-324:LYS:HE2	1.98	0.46
1:A:464:ALA:HB3	1:A:465:PRO:HD3	1.97	0.46
1:B:-219:LEU:HD12	1:B:-165:ASN:O	2.16	0.46
1:A:475:ASN:HB3	1:A:700:SER:OG	2.16	0.46
1:B:-359:ILE:HG13	1:B:-358:ASN:N	2.31	0.46
2:B:801:ADP:N7	4:B:913:HOH:O	2.36	0.45
1:A:390:GLU:N	1:A:704:ASN:OD1	2.50	0.45
1:B:423:ILE:HD11	1:B:441:SER:HB3	1.99	0.45
1:A:448:CYS:O	1:A:449:HIS:O	2.34	0.45
1:A:467:LEU:HB2	1:A:505:PHE:CE1	2.52	0.45
1:B:399:ARG:HA	1:B:442:PHE:O	2.16	0.45
1:B:398:VAL:HG21	1:B:438:TYR:CE2	2.51	0.45
1:A:443:TRP:CE2	1:A:445:PHE:HB3	2.51	0.45
1:A:399:ARG:HA	1:A:442:PHE:O	2.16	0.45
1:A:724:LEU:O	1:A:728:ARG:HG3	2.17	0.45
1:A:607:SER:OG	1:A:638:ASP:HB3	2.17	0.45
1:B:491:THR:HG21	1:B:710:ILE:HD12	1.98	0.45
1:A:491:THR:HG21	1:A:710:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-208:ALA:HB3	1:B:-114:LYS:HB2	1.99	0.44
1:A:-327:LEU:HA	1:A:-324:LYS:HG2	2.00	0.44
1:A:423:ILE:HD11	1:A:441:SER:HB3	1.99	0.44
1:B:607:SER:OG	1:B:638:ASP:HB3	2.18	0.44
1:A:-253:TYR:CZ	1:A:-245:PRO:HG3	2.53	0.44
1:A:647:THR:OG1	1:A:648:ALA:N	2.49	0.44
1:A:398:VAL:HG21	1:A:438:TYR:CE2	2.52	0.44
1:A:-219:LEU:HD12	1:A:-165:ASN:O	2.18	0.44
1:A:555:ARG:NH2	1:A:567:GLU:OE1	2.51	0.44
1:B:467:LEU:HB2	1:B:505:PHE:CE1	2.53	0.44
1:A:509:LEU:HD11	1:A:613:MET:CE	2.47	0.44
1:B:-18:SER:HB2	1:B:-16:ARG:H	1.83	0.44
1:B:733:ALA:O	1:B:734:ARG:CB	2.66	0.44
1:A:476:THR:HG22	1:A:706:LYS:HB2	2.00	0.44
1:B:531:GLU:HG3	1:B:605:SER:OG	2.18	0.43
1:B:731:THR:O	1:B:734:ARG:N	2.47	0.43
1:A:-327:LEU:HD12	1:A:-326:GLU:N	2.33	0.43
1:B:724:LEU:O	1:B:728:ARG:HG3	2.18	0.43
1:B:443:TRP:CE2	1:B:445:PHE:HB3	2.53	0.43
1:B:469:ARG:HD2	1:B:706:LYS:HE3	2.00	0.43
1:B:462:LEU:HD23	1:B:710:ILE:HD11	2.00	0.43
1:A:618:THR:CB	1:A:627:ASP:HB3	2.49	0.43
1:A:-189:VAL:HB	1:A:-5:GLN:NE2	2.34	0.43
1:B:-351:GLY:O	1:B:-348:GLU:HB2	2.18	0.43
1:B:-242:THR:HB	1:B:-239:GLU:HG3	2.00	0.43
1:B:733:ALA:C	1:B:734:ARG:HG2	2.39	0.42
1:B:401:ARG:HB2	1:B:402:PRO:CD	2.49	0.42
1:A:-242:THR:HB	1:A:-239:GLU:HG3	2.02	0.42
1:A:-327:LEU:C	1:A:-327:LEU:HD12	2.39	0.42
1:B:464:ALA:HB3	1:B:465:PRO:HD3	2.00	0.42
1:A:-53:ILE:O	1:A:-52:ALA:C	2.58	0.42
1:B:-173:ASP:O	1:B:-172:LEU:C	2.56	0.42
1:A:-261:ALA:HA	1:A:-68:VAL:HA	2.01	0.42
1:B:725:SER:HB3	4:B:903:HOH:O	2.20	0.42
1:B:-253:TYR:CZ	1:B:-245:PRO:HG3	2.55	0.42
1:A:449:HIS:CD2	1:A:451:GLY:H	2.38	0.42
1:A:-253:TYR:CE2	1:A:-245:PRO:HG3	2.55	0.42
1:B:-253:TYR:CE2	1:B:-245:PRO:HG3	2.55	0.42
1:B:449:HIS:CG	1:B:450:PRO:CD	3.03	0.41
1:B:488:LYS:N	2:B:801:ADP:O1A	2.52	0.41
1:B:-261:ALA:HA	1:B:-68:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-280:TYR:O	1:B:-277:THR:OG1	2.31	0.41
1:B:537:ILE:HD13	1:B:566:VAL:HG22	2.02	0.41
1:A:-91:PHE:O	1:A:-87:TYR:HB2	2.20	0.41
1:B:644:ARG:HG2	1:B:722:GLU:OE1	2.20	0.41
1:B:-91:PHE:O	1:B:-87:TYR:HB2	2.20	0.41
1:A:-342:GLU:O	1:A:-338:GLY:N	2.54	0.41
1:B:-212:TRP:CD1	1:B:-112:PHE:CE2	3.08	0.41
1:B:-330:PRO:HD2	1:B:-327:LEU:HD12	2.02	0.41
1:A:401:ARG:HB2	1:A:402:PRO:CD	2.50	0.41
1:B:-53:ILE:O	1:B:-52:ALA:C	2.60	0.41
1:A:-116:PRO:O	1:A:-114:LYS:HD2	2.21	0.41
1:A:537:ILE:HD13	1:A:566:VAL:HG22	2.03	0.40
1:B:-238:ILE:N	1:B:-237:PRO:CD	2.83	0.40
1:A:559:HIS:CD2	1:A:560:PRO:HD2	2.56	0.40
1:A:618:THR:HB	1:A:627:ASP:HB3	2.04	0.40
1:A:-329:ASP:O	1:A:-327:LEU:N	2.55	0.40
1:A:-212:TRP:CD1	1:A:-112:PHE:CE2	3.09	0.40
1:A:673:SER:HB2	1:A:732:GLN:OE1	2.22	0.40
1:B:652:GLY:O	1:B:654:ARG:N	2.54	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	673/720 (94%)	634 (94%)	33 (5%)	6 (1%)	21	47
1	B	677/720 (94%)	643 (95%)	30 (4%)	4 (1%)	30	58
All	All	1350/1440 (94%)	1277 (95%)	63 (5%)	10 (1%)	26	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	CYS
1	A	449	HIS
1	B	-328	LYS
1	B	653	GLN
1	A	-192	ILE
1	A	447	GLU
1	B	-192	ILE
1	B	-58	ALA
1	A	-328	LYS
1	A	-58	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	A	500/596 (84%)	464 (93%)	36 (7%)	18	40
1	B	500/596 (84%)	474 (95%)	26 (5%)	29	56
All	All	1000/1192 (84%)	938 (94%)	62 (6%)	23	48

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-352	ASN
1	A	-327	LEU
1	A	-324	LYS
1	A	-315	ASP
1	A	-297	SER
1	A	-282	LYS
1	A	-259	GLU
1	A	-256	SER
1	A	-248	LEU
1	A	-225	SER
1	A	-175	LEU
1	A	-143	ASN
1	A	-130	VAL
1	A	-95	LEU

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Mol	Chain	Res	Type
1	A	-79	GLU
1	A	400	VAL
1	A	419	ASN
1	A	448	CYS
1	A	486	SER
1	A	488	LYS
1	A	495	LEU
1	A	498	GLU
1	A	522	SER
1	A	570	SER
1	A	589	LYS
1	A	604	ARG
1	A	618	THR
1	A	647	THR
1	A	654	ARG
1	A	683	ARG
1	A	684	VAL
1	A	700	SER
1	A	707	THR
1	A	718	SER
1	A	725	SER
1	A	732	GLN
1	B	-329	ASP
1	B	-315	ASP
1	B	-297	SER
1	B	-270	ASN
1	B	-266	ILE
1	B	-259	GLU
1	B	-256	SER
1	B	-225	SER
1	B	-175	LEU
1	B	-143	ASN
1	B	-141	PRO
1	B	-130	VAL
1	B	421	GLU
1	B	486	SER
1	B	488	LYS
1	B	495	LEU
1	B	522	SER
1	B	570	SER
1	B	591	ARG
1	B	618	THR

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Mol	Chain	Res	Type
1	B	657	GLU
1	B	710	ILE
1	B	718	SER
1	B	725	SER
1	B	732	GLN
1	B	734	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-352	ASN
1	A	427	HIS
1	A	449	HIS
1	A	635	ASN
1	B	-197	ASN
1	B	449	HIS

### 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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	A	801	-	22,29,29	1.44	3 (13%)	27,45,45	2.74	8 (29%)
3	EDO	A	802	-	3,3,3	0.76	0	2,2,2	0.39	0
2	ADP	B	801	-	22,29,29	1.47	3 (13%)	27,45,45	2.22	6 (22%)
3	EDO	B	802	-	3,3,3	0.90	0	2,2,2	0.48	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	-	-	0/12/32/32	0/3/3/3
3	EDO	A	802	-	-	0/1/1/1	0/0/0/0
2	ADP	B	801	-	-	0/12/32/32	0/3/3/3
3	EDO	B	802	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ADP	C5-C4	2.55	1.46	1.40
2	A	801	ADP	C5-C4	2.70	1.46	1.40
2	B	801	ADP	C2-N3	2.84	1.37	1.32
2	A	801	ADP	C2-N3	2.88	1.37	1.32
2	A	801	ADP	O4'-C1'	3.14	1.45	1.41
2	B	801	ADP	O4'-C1'	3.82	1.46	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	N3-C2-N1	-9.45	121.66	128.89
2	B	801	ADP	PA-O3A-PB	-6.69	110.23	132.67
2	B	801	ADP	N3-C2-N1	-5.79	124.46	128.89
2	A	801	ADP	PA-O3A-PB	-5.69	113.59	132.67
2	A	801	ADP	C4-C5-N7	-3.66	106.11	109.48
2	A	801	ADP	C2'-C1'-N9	-3.47	108.99	114.29
2	B	801	ADP	C2'-C1'-N9	-3.37	109.14	114.29
2	A	801	ADP	C1'-N9-C4	-2.04	123.86	126.94
2	B	801	ADP	O2A-PA-O1A	2.00	123.37	112.53
2	A	801	ADP	O3B-PB-O1B	2.24	117.78	110.58
2	B	801	ADP	N6-C6-N1	2.26	124.05	119.20
2	A	801	ADP	O3A-PA-O5'	2.88	110.59	102.94
2	A	801	ADP	C4'-O4'-C1'	3.17	113.21	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ADP	O3A-PA-O5'	3.95	113.41	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	1	0
2	B	801	ADP	5	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	683/720 (94%)	0.10	11 (1%) 74 75	29, 45, 84, 120	0
1	B	687/720 (95%)	0.07	13 (1%) 70 71	31, 46, 73, 98	0
All	All	1370/1440 (95%)	0.08	24 (1%) 71 72	29, 46, 79, 120	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	PRO	4.4
1	B	600	ASP	4.4
1	A	646	SER	3.8
1	A	-101	ALA	3.6
1	B	-290	THR	3.0
1	B	-318	ALA	3.0
1	B	-316	GLY	2.7
1	A	625	GLU	2.7
1	A	645	CYS	2.6
1	B	-296	GLY	2.6
1	B	-101	ALA	2.5
1	B	-315	ASP	2.5
1	B	543	CYS	2.4
1	A	542	VAL	2.3
1	A	480	ALA	2.3
1	B	480	ALA	2.2
1	B	-347	VAL	2.2
1	B	-340	ASP	2.1
1	A	-229	ALA	2.1
1	A	648	ALA	2.1
1	B	-102	ALA	2.1
1	A	618	THR	2.0
1	B	645	CYS	2.0
1	A	647	THR	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( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	802	4/4	0.91	0.20	0.78	17,18,18,19	0
3	EDO	B	802	4/4	0.90	0.15	-0.56	17,18,19,19	0
2	ADP	B	801	27/27	0.94	0.15	-0.88	15,18,20,21	0
2	ADP	A	801	27/27	0.94	0.13	-1.28	14,18,20,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.