



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:45 AM GMT

PDB ID : 2Y65
Title : Crystal structure of Drosophila melanogaster kinesin-1 motor domain dimer-tail complex
Authors : Kaan, H.Y.K.; Hackney, D.D.; Kozielski, F.
Deposited on : 2011-01-19
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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (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

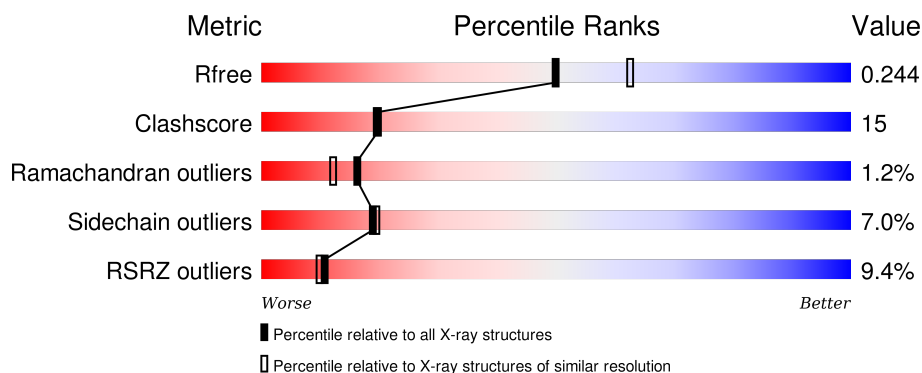
1 Overall quality at a glance

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 ≥ 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	365	<div> <div>6%</div> <div>67% 19% • • 10%</div> </div>
1	B	365	<div> <div>7%</div> <div>65% 25% • 7%</div> </div>
1	C	365	<div> <div>10%</div> <div>73% 18% • 6%</div> </div>
1	D	365	<div> <div>11%</div> <div>69% 21% • 7%</div> </div>
2	W	20	<div> <div>10%</div> <div>10% 35% 20% 35%</div> </div>

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Mol	Chain	Length	Quality of chain
2	X	20	<div><div></div><div></div><div></div><div></div><div></div></div> <div>15%40%20%5%35%</div>
2	Y	20	<div><div></div><div></div><div></div><div></div><div></div></div> <div>10%45%5%10%40%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11750 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 KINESIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	10	0
			2598	1640	450	499	9			
1	B	341	Total	C	N	O	S	0	6	0
			2681	1692	460	519	10			
1	C	343	Total	C	N	O	S	0	3	0
			2694	1693	471	521	9			
1	D	338	Total	C	N	O	S	0	6	0
			2654	1672	457	516	9			

- Molecule 2 is a protein called KINESIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	W	13	Total	C	N	O	0	13	0
			174	108	36	30			
2	X	13	Total	C	N	O	0	0	0
			93	58	19	16			
2	Y	12	Total	C	N	O	0	0	0
			88	55	18	15			

There are 12 discrepancies between the modelled and reference sequences:

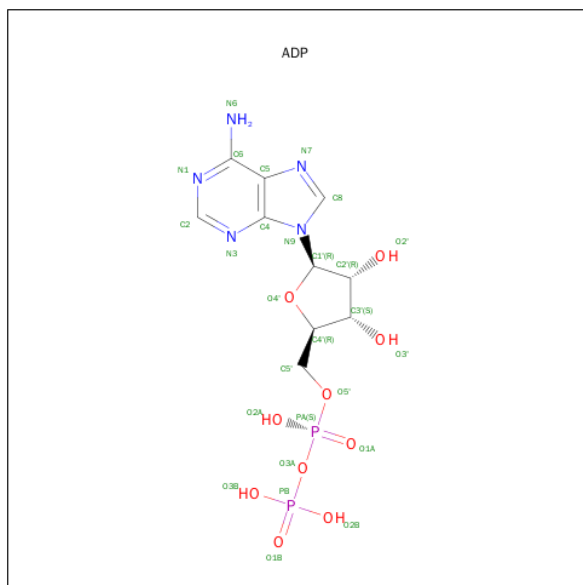
Chain	Residue	Modelled	Actual	Comment	Reference
W	935	GLY	-	EXPRESSION TAG	UNP P17210
W	936	SER	-	EXPRESSION TAG	UNP P17210
W	953	THR	-	EXPRESSION TAG	UNP P17210
W	954	SER	-	EXPRESSION TAG	UNP P17210
X	935	GLY	-	EXPRESSION TAG	UNP P17210
X	936	SER	-	EXPRESSION TAG	UNP P17210
X	953	THR	-	EXPRESSION TAG	UNP P17210
X	954	SER	-	EXPRESSION TAG	UNP P17210
Y	935	GLY	-	EXPRESSION TAG	UNP P17210
Y	936	SER	-	EXPRESSION TAG	UNP P17210

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	953	THR	-	EXPRESSION TAG	UNP P17210
Y	954	SER	-	EXPRESSION TAG	UNP P17210

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



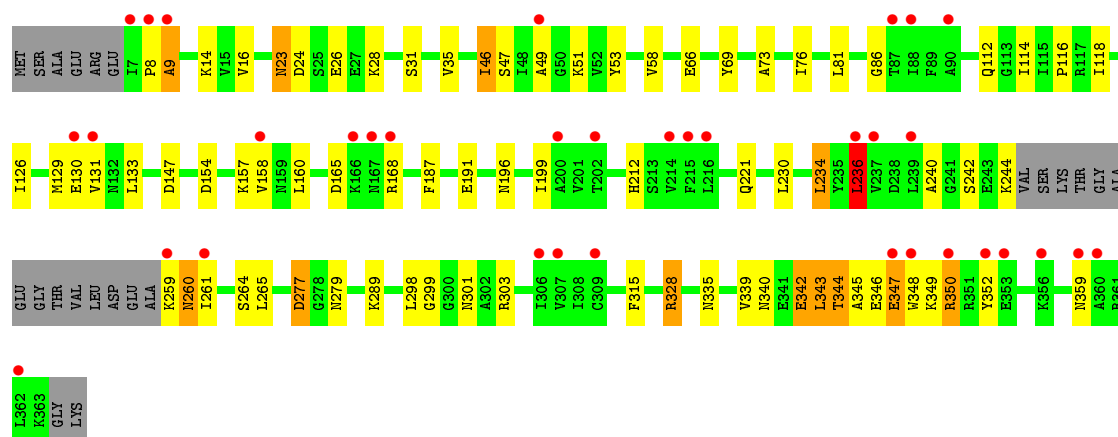
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

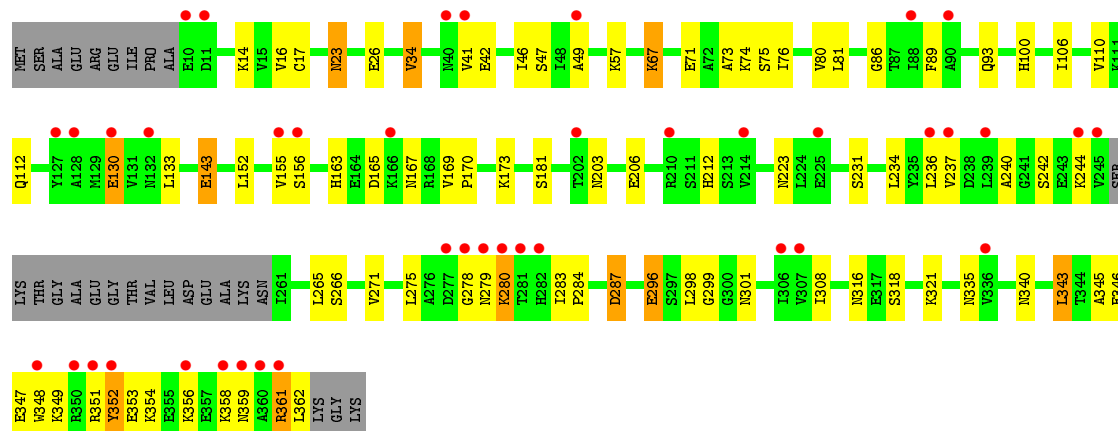
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

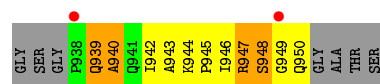
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	196	Total 196	O 196	0	0
5	B	175	Total 175	O 175	0	0
5	C	180	Total 180	O 180	0	0
5	D	96	Total 96	O 96	0	0
5	W	2	Total 2	O 2	0	0
5	X	6	Total 6	O 6	0	0
5	Y	1	Total 1	O 1	0	0



• Molecule 1: KINESIN HEAVY CHAIN



• Molecule 2: KINESIN HEAVY CHAIN



• Molecule 2: KINESIN HEAVY CHAIN



• Molecule 2: KINESIN HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.77Å 190.71Å 145.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 29.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.20) 99.9 (29.74-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.252 0.188 , 0.244	Depositor DCC
R_{free} test set	4044 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.011 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 80446 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11750	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8708e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: MG, 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	0/2669	0.90	1/3604 (0.0%)
1	B	0.57	0/2741	0.84	2/3699 (0.1%)
1	C	0.59	0/2745	0.89	5/3702 (0.1%)
1	D	0.48	0/2713	0.77	0/3661
2	W	0.34	0/174	0.76	0/229
2	X	0.37	0/94	0.60	0/125
2	Y	0.47	0/89	0.80	0/118
All	All	0.56	0/11225	0.85	8/15138 (0.1%)

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	D	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	236	LEU	CB-CG-CD1	6.36	121.81	111.00
1	A	16	VAL	CG1-CB-CG2	5.93	120.39	110.90
1	C	16	VAL	CG1-CB-CG2	5.90	120.34	110.90
1	B	133	LEU	CA-CB-CG	5.40	127.73	115.30
1	C	234	LEU	CB-CG-CD2	-5.39	101.84	111.00
1	C	328	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	234	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	49	ALA	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	2598	0	2613	77	0
1	B	2681	0	2663	79	0
1	C	2694	0	2679	76	0
1	D	2654	0	2637	79	0
2	W	174	0	188	29	0
2	X	93	0	98	7	0
2	Y	88	0	96	4	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	196	0	0	9	0
5	B	175	0	0	8	0
5	C	180	0	0	6	0
5	D	96	0	0	9	0
5	W	2	0	0	0	0
5	X	6	0	0	4	0
5	Y	1	0	0	0	0
All	All	11750	0	11022	330	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 15.

All (330) 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:168:ARG:HH11	1:A:168:ARG:HG3	1.04	1.18
2:W:943[A]:ALA:HB3	2:W:944[A]:LYS:CG	1.79	1.12
2:W:945[B]:PRO:C	2:W:946[B]:ILE:HD13	1.74	1.07
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:HA	1.30	1.07
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:HG2	1.88	1.03
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:CG	2.39	0.99
2:W:943[A]:ALA:HB3	2:W:944[A]:LYS:HG3	1.43	0.98
2:X:947:ARG:NH1	5:X:2004:HOH:O	1.94	0.98
1:D:80:VAL:HG21	1:D:234[B]:LEU:HD21	1.46	0.98
1:D:80:VAL:HG21	1:D:234[B]:LEU:CD2	1.95	0.96
1:C:46[A]:ILE:HD13	1:C:46[A]:ILE:H	1.32	0.94
1:B:39:ASN:H	1:C:196:ASN:HD21	1.17	0.92
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:CA	1.99	0.92
1:D:343:LEU:H	1:D:343:LEU:HD12	1.32	0.92
1:A:168:ARG:HG3	1:A:168:ARG:NH1	1.77	0.92
1:C:348:TRP:CD1	1:D:345:ALA:HB1	2.06	0.91
1:D:299:GLY:H	1:D:335:ASN:HD21	1.16	0.89
2:W:943[A]:ALA:HB3	2:W:944[A]:LYS:HG2	1.48	0.88
2:W:939[B]:GLN:HG3	2:W:940[B]:ALA:H	1.39	0.86
2:W:947[B]:ARG:O	2:W:948[B]:SER:OG	1.94	0.85
1:A:167:ASN:N	1:A:168:ARG:HA	1.91	0.84
1:C:343:LEU:HD23	1:C:347:GLU:HB3	1.59	0.84
1:D:100:HIS:HD2	5:D:2094:HOH:O	1.60	0.84
1:C:348:TRP:HD1	1:D:345:ALA:HB1	1.40	0.83
1:C:212:HIS:CD2	1:C:240:ALA:H	1.98	0.81
1:A:262:ASN:HD21	1:A:264:SER:HB2	1.44	0.81
1:B:51:LYS:HE2	1:B:328:ARG:HH22	1.44	0.81
1:C:187:PHE:O	1:C:191[A]:GLU:HG2	1.80	0.80
1:C:46[A]:ILE:HD11	1:C:53:TYR:HB2	1.64	0.80
1:A:299:GLY:H	1:A:335:ASN:HD21	1.26	0.79
1:C:299:GLY:H	1:C:335:ASN:HD21	1.29	0.78
1:C:259:LYS:O	1:C:260:ASN:HB2	1.81	0.78
1:A:74:LYS:O	1:A:77[B]:VAL:HG12	1.83	0.78
1:D:80:VAL:CG2	1:D:234[B]:LEU:HD21	2.14	0.78
1:A:162:VAL:HG11	1:A:292:ARG:HG2	1.65	0.77
1:A:73:ALA:O	1:A:76:ILE:HG22	1.84	0.76
1:C:51:LYS:HE2	1:C:328:ARG:HH22	1.51	0.76
1:B:299:GLY:H	1:B:335:ASN:ND2	1.83	0.75
1:B:181:SER:HB3	2:X:944:LYS:HG3	1.68	0.75
1:D:181:SER:HB3	2:W:943[A]:ALA:HB2	1.67	0.75
1:D:106:ILE:O	5:D:2048:HOH:O	2.05	0.74
1:C:342:GLU:O	5:C:2172:HOH:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ASN:HD21	1:C:340:ASN:HD21	1.35	0.73
1:A:23:ASN:C	1:A:23:ASN:HD22	1.91	0.73
1:D:41:VAL:HG22	1:D:42:GLU:O	1.88	0.73
1:D:57:LYS:NZ	1:D:71:GLU:HG3	2.03	0.73
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:CA	2.66	0.72
1:D:343:LEU:HD12	1:D:343:LEU:N	2.03	0.72
1:D:353:GLU:HB3	5:D:2090:HOH:O	1.87	0.72
1:A:158:VAL:O	5:A:2108:HOH:O	2.08	0.72
1:D:299:GLY:H	1:D:335:ASN:ND2	1.87	0.71
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:HG2	1.72	0.71
1:A:345:ALA:HB1	1:A:349:LYS:HG3	1.73	0.71
1:B:262:ASN:HD21	1:B:264:SER:HB2	1.55	0.71
1:C:31:SER:OG	1:C:315:PHE:HB2	1.91	0.71
1:C:299:GLY:H	1:C:335:ASN:ND2	1.89	0.71
1:C:344:THR:CG2	1:C:347:GLU:HB2	2.21	0.70
1:B:299:GLY:H	1:B:335:ASN:HD21	1.36	0.70
2:W:939[B]:GLN:O	2:W:940[B]:ALA:HB3	1.92	0.70
1:A:196:ASN:ND2	5:A:2136:HOH:O	2.25	0.70
1:D:57:LYS:HZ1	1:D:71:GLU:HG3	1.57	0.69
1:B:23:ASN:HD22	1:B:23:ASN:C	1.95	0.69
1:D:112:GLN:NE2	5:D:2048:HOH:O	2.24	0.69
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:CG	2.21	0.69
1:A:165:ASP:OD1	1:A:168:ARG:O	2.11	0.68
1:B:262:ASN:HD21	1:B:264:SER:CB	2.07	0.68
1:C:343:LEU:CD2	1:C:347:GLU:HB3	2.23	0.68
1:A:280:LYS:HD2	1:A:281:THR:H	1.60	0.67
1:C:154:ASP:OD2	1:C:157:LYS:HE3	1.95	0.67
1:C:66:GLU:OE2	5:C:2049:HOH:O	2.12	0.67
2:X:947:ARG:NH2	5:X:2006:HOH:O	2.22	0.67
1:C:344:THR:HG22	1:C:347:GLU:HB2	1.75	0.67
1:C:46[B]:ILE:HG12	1:C:47:SER:N	2.09	0.67
1:C:23:ASN:ND2	1:C:26:GLU:H	1.92	0.66
1:A:57:LYS:HG2	1:A:71[B]:GLU:HG2	1.77	0.66
1:B:45[B]:CYS:SG	1:B:52:VAL:HG13	2.36	0.66
1:B:267:ALA:O	1:B:271:VAL:HG23	1.95	0.66
1:D:354:LYS:O	1:D:358:LYS:HB2	1.94	0.66
1:C:328:ARG:HD2	5:C:2166:HOH:O	1.96	0.66
1:D:100:HIS:CD2	5:D:2094:HOH:O	2.42	0.65
1:A:299:GLY:H	1:A:335:ASN:ND2	1.92	0.65
2:W:946[B]:ILE:HD13	2:W:946[B]:ILE:N	2.12	0.65
1:B:23:ASN:ND2	1:B:26:GLU:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLN:HG3	1:B:350:ARG:HH22	1.62	0.64
1:C:277:ASP:HB3	1:C:279:ASN:ND2	2.12	0.64
1:A:11:ASP:OD2	1:A:303[B]:ARG:HD2	1.97	0.63
1:A:317:GLU:OE1	5:A:2175:HOH:O	2.14	0.63
1:A:212:HIS:CD2	1:A:240:ALA:H	2.16	0.63
1:A:16:VAL:HG22	1:A:57:LYS:HB3	1.81	0.63
1:A:301:ASN:HD21	1:A:340:ASN:HD21	1.46	0.63
1:B:39:ASN:H	1:C:196:ASN:ND2	1.94	0.63
1:A:23:ASN:ND2	1:A:26:GLU:H	1.96	0.63
2:W:945[B]:PRO:O	2:W:946[B]:ILE:HD13	1.98	0.62
1:B:212:HIS:CD2	1:B:240:ALA:H	2.17	0.62
1:B:299:GLY:HA2	1:B:335:ASN:HD22	1.65	0.62
1:B:11:ASP:OD2	1:B:303:ARG:HG2	1.99	0.62
1:A:112:GLN:NE2	5:A:2089:HOH:O	2.33	0.61
2:W:939[B]:GLN:O	2:W:940[B]:ALA:CB	2.48	0.61
1:D:343:LEU:CD1	1:D:343:LEU:H	2.09	0.61
1:C:51:LYS:HE2	1:C:328:ARG:NH2	2.15	0.61
1:A:168:ARG:HG3	1:A:169:VAL:H	1.65	0.61
1:D:345:ALA:O	1:D:347:GLU:N	2.34	0.61
1:A:168:ARG:HH11	1:A:168:ARG:CG	1.93	0.60
1:B:45[B]:CYS:SG	1:B:52:VAL:CG1	2.89	0.60
1:C:51:LYS:CE	1:C:328:ARG:HH22	2.13	0.60
1:B:73:ALA:O	1:B:76:ILE:HG22	2.02	0.59
1:A:93:GLN:HE22	1:A:316:ASN:HB3	1.66	0.59
1:C:35:VAL:HG13	1:C:46[B]:ILE:HG13	1.85	0.59
1:C:23:ASN:HD22	1:C:23:ASN:C	2.06	0.59
1:D:23:ASN:ND2	1:D:26:GLU:H	2.00	0.59
1:D:23:ASN:C	1:D:23:ASN:HD22	2.06	0.59
1:C:147:ASP:O	1:C:289:LYS:HE3	2.03	0.59
1:C:259:LYS:O	1:C:260:ASN:CB	2.50	0.59
1:A:179:PHE:CE1	2:Y:945:PRO:HG2	2.38	0.58
1:A:339:VAL:HG12	5:A:2184:HOH:O	2.03	0.58
1:C:244:LYS:HA	1:C:260:ASN:HA	1.85	0.58
1:B:299:GLY:N	1:B:335:ASN:ND2	2.50	0.58
1:A:80[B]:VAL:HG21	1:A:234[B]:LEU:HG	1.86	0.58
1:D:80:VAL:CG2	1:D:234[B]:LEU:CD2	2.78	0.58
1:C:165:ASP:HB2	5:C:2103:HOH:O	2.04	0.58
1:D:163:HIS:O	1:D:170:PRO:HA	2.02	0.58
1:D:143:GLU:HG2	1:D:152:LEU:HD21	1.86	0.57
1:C:348:TRP:HD1	1:D:345:ALA:CB	2.15	0.57
1:A:234[A]:LEU:CD2	1:A:236:LEU:HD21	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:SER:HA	1:D:265:LEU:HD13	1.87	0.57
1:D:345:ALA:C	1:D:347:GLU:H	2.07	0.57
1:D:16:VAL:HG22	1:D:57:LYS:HB2	1.86	0.57
1:B:73:ALA:O	1:B:74:LYS:C	2.42	0.57
1:A:234[A]:LEU:HD21	1:A:236:LEU:HD21	1.86	0.57
1:C:46[A]:ILE:HG23	1:C:58:VAL:HG11	1.87	0.56
1:C:301:ASN:ND2	1:C:340:ASN:HD21	2.02	0.56
1:D:181:SER:HB3	2:W:943[A]:ALA:CB	2.33	0.56
1:D:106:ILE:HG12	5:D:2049:HOH:O	2.04	0.56
1:C:277:ASP:HB3	1:C:279:ASN:HD21	1.69	0.56
1:B:29:ALA:O	1:B:315[B]:PHE:HE2	1.87	0.56
1:D:80:VAL:HG21	1:D:234[B]:LEU:CG	2.35	0.56
1:B:23:ASN:HD22	1:B:26:GLU:H	1.51	0.56
1:A:100:HIS:HD2	5:A:2188:HOH:O	1.89	0.56
2:W:939[B]:GLN:HG3	2:W:940[B]:ALA:N	2.17	0.56
1:D:279:ASN:O	1:D:280:LYS:HB2	2.05	0.56
1:A:198:HIS:HD2	1:B:111:LYS:NZ	2.05	0.55
2:W:943[A]:ALA:HB1	2:W:944[A]:LYS:CB	2.36	0.55
2:W:942[A]:ILE:HG22	2:W:943[A]:ALA:N	2.21	0.55
1:A:158:VAL:CG1	5:A:2109:HOH:O	2.55	0.55
1:C:114:ILE:O	1:C:118:ILE:HG12	2.06	0.55
1:B:244:LYS:HA	1:B:260:ASN:O	2.07	0.55
1:D:212:HIS:CD2	1:D:240:ALA:H	2.24	0.54
1:D:133:LEU:HD23	1:D:223:ASN:HA	1.90	0.54
1:C:242:SER:HA	1:C:265:LEU:HD13	1.88	0.54
1:B:69:TYR:HE1	1:B:118:ILE:HG13	1.71	0.54
1:C:342:GLU:HG2	5:C:2135:HOH:O	2.07	0.54
1:C:212:HIS:HE1	1:C:264:SER:OG	1.91	0.54
1:C:69:TYR:HE1	1:C:118:ILE:HD13	1.72	0.54
1:B:343:LEU:HD13	1:B:347:GLU:HG3	1.90	0.54
2:X:946:ILE:N	2:X:946:ILE:HD13	2.22	0.54
1:D:343:LEU:CD2	1:D:351:ARG:HH12	2.21	0.53
1:A:345:ALA:O	1:A:349:LYS:N	2.27	0.53
1:D:93:GLN:HE22	1:D:316:ASN:HB3	1.72	0.53
1:D:296[A]:GLU:HG3	1:D:301:ASN:H	1.73	0.53
1:C:349:LYS:HB2	1:D:348:TRP:CE2	2.42	0.53
1:A:158:VAL:HG12	1:A:159:ASN:H	1.73	0.53
1:B:233:LYS:HE3	5:B:2132:HOH:O	2.09	0.53
1:B:346[A]:GLU:CD	1:B:346[A]:GLU:H	2.10	0.52
1:B:39:ASN:N	1:C:196:ASN:HD21	1.96	0.52
1:D:284:PRO:HB2	1:D:287:ASP:OD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:PHE:HB3	1:D:237:VAL:HB	1.91	0.52
1:B:299:GLY:HA2	1:B:335:ASN:ND2	2.25	0.52
1:B:182:SER:HB2	1:B:183:PRO:HD2	1.92	0.52
1:B:170:PRO:HG2	1:B:295:GLN:HG2	1.92	0.51
1:A:184:GLU:O	1:A:188:GLU:HG3	2.09	0.51
1:D:361:ARG:O	1:D:362:LEU:C	2.49	0.51
1:A:280:LYS:HD2	1:A:281:THR:N	2.26	0.51
1:C:157:LYS:HB3	1:C:160:LEU:HD21	1.91	0.51
1:D:155:VAL:O	1:D:155:VAL:HG22	2.11	0.51
1:B:133:LEU:HD12	1:B:223:ASN:HA	1.92	0.51
1:C:212:HIS:HD2	1:C:240:ALA:H	1.52	0.51
1:D:352:TYR:CE2	1:D:353:GLU:HG3	2.45	0.50
1:B:34:VAL:HG22	1:B:34:VAL:O	2.10	0.50
1:D:75:SER:OG	5:D:2039:HOH:O	2.19	0.50
1:D:100:HIS:HE1	5:D:2003:HOH:O	1.93	0.50
1:C:46[A]:ILE:CD1	1:C:53:TYR:HB2	2.40	0.50
1:B:301:ASN:ND2	1:B:340:ASN:HD21	2.10	0.50
1:A:168:ARG:HH11	1:A:169:VAL:H	1.58	0.50
2:X:947:ARG:NE	5:X:2003:HOH:O	2.43	0.50
1:B:163:HIS:CD2	1:B:173:LYS:HD2	2.47	0.50
2:W:942[A]:ILE:HG22	2:W:943[A]:ALA:HB2	1.94	0.49
1:C:73:ALA:O	1:C:76:ILE:HG22	2.11	0.49
1:B:48:ILE:HD11	1:B:317:GLU:HG3	1.95	0.49
1:D:359:ASN:HA	1:D:362:LEU:HD12	1.93	0.49
1:A:267:ALA:O	1:A:271:VAL:HG23	2.13	0.49
1:C:46[A]:ILE:HD13	1:C:53:TYR:O	2.12	0.49
1:C:346:GLU:O	1:C:349:LYS:HB3	2.13	0.49
2:W:949[B]:GLY:HA3	2:W:950[B]:GLN:HB2	1.94	0.49
1:A:23:ASN:HD22	1:A:26:GLU:H	1.61	0.49
1:A:19:PHE:CE2	1:A:35:VAL:HG21	2.48	0.49
1:A:262:ASN:HD22	1:A:265:LEU:H	1.60	0.48
1:C:46[A]:ILE:CG2	1:C:58:VAL:HG11	2.43	0.48
1:B:299:GLY:CA	1:B:335:ASN:ND2	2.76	0.48
1:A:158:VAL:HG12	1:A:159:ASN:N	2.28	0.48
1:B:22:LEU:HD23	1:B:27:GLU:HG3	1.95	0.48
1:A:9:ALA:HB1	1:A:337:VAL:O	2.13	0.48
1:C:126:ILE:O	1:C:129:MET:HB2	2.14	0.48
1:A:158:VAL:HG13	5:A:2109:HOH:O	2.12	0.48
1:B:262:ASN:HB2	5:B:2049:HOH:O	2.12	0.48
1:B:242:SER:HA	1:B:265:LEU:HD13	1.95	0.48
1:A:111:LYS:NZ	1:B:198:HIS:HD2	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ASN:HD22	1:D:206:GLU:HB2	1.78	0.48
1:A:301:ASN:ND2	1:A:340:ASN:HD21	2.12	0.48
1:B:165:ASP:OD2	1:B:169:VAL:HG23	2.13	0.48
1:C:24:ASP:OD1	1:C:28:LYS:HE3	2.14	0.47
2:X:948:SER:OG	2:X:948:SER:O	2.32	0.47
1:D:278:GLY:HA2	5:D:2079:HOH:O	2.12	0.47
1:B:301:ASN:HD21	1:B:340:ASN:HD21	1.62	0.47
1:A:227:GLN:HB3	1:A:344:THR:HG21	1.96	0.47
1:D:271:VAL:O	1:D:275:LEU:HD12	2.15	0.47
1:A:168:ARG:HG3	1:A:169:VAL:N	2.28	0.47
1:D:17:CYS:HA	1:D:308:ILE:HG13	1.97	0.47
1:B:150:ARG:HD2	1:B:155:VAL:HB	1.96	0.47
1:A:168:ARG:C	1:A:169:VAL:HG13	2.35	0.47
1:D:352:TYR:CD1	1:D:356:LYS:HD3	2.49	0.47
1:D:34:VAL:HG13	1:D:34:VAL:O	2.15	0.47
2:W:946[B]:ILE:N	2:W:946[B]:ILE:CD1	2.76	0.47
1:D:57:LYS:HZ2	1:D:71:GLU:HG3	1.79	0.47
1:A:179:PHE:CD1	2:Y:945:PRO:HD2	2.50	0.47
1:D:296[A]:GLU:HG3	1:D:301:ASN:N	2.30	0.46
1:C:344:THR:HG23	1:C:347:GLU:HB2	1.97	0.46
1:B:299:GLY:N	1:B:335:ASN:HD21	2.09	0.46
1:B:275:LEU:HD11	1:B:298:LEU:O	2.13	0.46
1:D:67:LYS:HA	1:D:67:LYS:CE	2.45	0.46
1:A:262:ASN:ND2	1:A:264:SER:HB2	2.22	0.46
1:B:170:PRO:HG3	1:B:295:GLN:OE1	2.16	0.46
2:W:947[B]:ARG:C	2:W:948[B]:SER:OG	2.52	0.46
1:D:67:LYS:HA	1:D:67:LYS:HE3	1.97	0.46
1:A:286:ARG:HB2	5:A:2166:HOH:O	2.15	0.46
1:A:168:ARG:CG	1:A:168:ARG:NH1	2.59	0.46
1:A:177:GLU:H	2:Y:947:ARG:NH2	2.14	0.46
1:A:51:LYS:HE3	1:A:51:LYS:HB3	1.63	0.45
1:C:112:GLN:HB2	1:C:116:PRO:HG2	1.98	0.45
1:B:23:ASN:ND2	1:B:23:ASN:C	2.67	0.45
1:D:275:LEU:HG	1:D:283:ILE:HD12	1.97	0.45
1:C:359:ASN:HB2	1:D:359:ASN:OD1	2.16	0.45
1:D:73:ALA:O	1:D:74:LYS:C	2.53	0.45
2:W:942[A]:ILE:CG2	2:W:943[A]:ALA:N	2.79	0.45
1:B:47:SER:HB2	1:B:52:VAL:HG22	1.97	0.45
1:B:78:THR:HG23	5:B:2038:HOH:O	2.16	0.45
1:B:198:HIS:HE1	5:B:2040:HOH:O	1.99	0.45
1:A:168:ARG:HH11	1:A:169:VAL:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:943[A]:ALA:CB	2:W:944[A]:LYS:HA	2.10	0.45
1:A:130:GLU:O	1:A:131:VAL:C	2.55	0.45
1:B:70:ASN:ND2	5:B:2035:HOH:O	2.24	0.45
1:B:112:GLN:NE2	5:B:2066:HOH:O	2.50	0.44
1:A:221:GLN:HG2	1:A:230:LEU:HB2	2.00	0.44
1:A:89:PHE:HB3	1:A:237:VAL:HB	1.99	0.44
1:C:349:LYS:HG2	1:C:350:ARG:HD3	1.99	0.44
1:D:165:ASP:CB	1:D:167:ASN:H	2.30	0.44
1:A:152:LEU:HA	1:A:152:LEU:HD23	1.77	0.44
1:D:23:ASN:HD22	1:D:26:GLU:H	1.63	0.44
1:C:234:LEU:HD11	1:C:236:LEU:HD11	1.99	0.44
1:B:51:LYS:CE	1:B:328:ARG:HH22	2.23	0.44
1:B:139[A]:VAL:HG21	1:B:215:PHE:CZ	2.53	0.44
1:C:221:GLN:HG2	1:C:230:LEU:HB2	2.00	0.44
2:X:942:ILE:HG22	2:X:942:ILE:O	2.18	0.44
1:B:280:LYS:HE3	1:B:282:HIS:O	2.18	0.44
1:B:86:GLY:O	1:B:234:LEU:HA	2.18	0.43
1:C:8:PRO:O	1:C:9:ALA:CB	2.66	0.43
1:D:80:VAL:HG21	1:D:234[B]:LEU:HG	2.00	0.43
1:C:345:ALA:HA	1:D:345:ALA:HB2	2.01	0.43
1:D:301:ASN:HD21	1:D:340:ASN:HD21	1.65	0.43
1:D:165:ASP:HB2	1:D:167:ASN:H	1.83	0.43
1:A:123:PHE:CG	1:A:183:PRO:HD3	2.53	0.43
1:A:244:LYS:HA	1:A:261:ILE:HG13	2.00	0.43
1:C:346:GLU:HB2	1:C:350:ARG:NH1	2.33	0.43
1:A:73:ALA:O	1:A:76:ILE:CG2	2.64	0.43
1:B:131:VAL:HG12	1:B:132:ASN:N	2.34	0.43
1:C:23:ASN:HD21	1:C:26:GLU:HG3	1.84	0.43
1:B:356:LYS:HB3	1:B:356:LYS:HE2	1.69	0.43
1:B:262:ASN:ND2	1:B:264:SER:CB	2.80	0.43
1:B:93:GLN:HE22	1:B:316:ASN:HB3	1.84	0.42
1:A:23:ASN:C	1:A:23:ASN:ND2	2.65	0.42
1:B:45[B]:CYS:HA	1:B:53:TYR:O	2.20	0.42
1:C:279:ASN:H	1:C:279:ASN:ND2	2.17	0.42
1:D:23:ASN:ND2	1:D:26:GLU:HG3	2.34	0.42
1:B:182:SER:HB2	1:B:183:PRO:CD	2.49	0.42
1:C:230:LEU:HD22	1:C:339:VAL:HG22	2.02	0.42
1:C:86:GLY:O	1:C:234:LEU:HA	2.20	0.42
1:C:349:LYS:HD3	1:D:348:TRP:CZ2	2.55	0.42
1:B:19:PHE:CE1	1:B:46:ILE:HG13	2.54	0.42
1:B:165:ASP:HB2	1:B:166:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:THR:O	1:C:345:ALA:C	2.57	0.42
1:B:343:LEU:HB2	1:B:348:TRP:NE1	2.35	0.42
1:B:20:ARG:O	1:B:312:PRO:HD3	2.20	0.42
1:A:168:ARG:NH1	1:A:169:VAL:H	2.18	0.42
1:D:352:TYR:CE1	1:D:356:LYS:HD3	2.55	0.42
1:B:316:ASN:ND2	5:B:2154:HOH:O	2.47	0.42
1:A:228:LYS:HE2	1:A:228:LYS:HB2	1.81	0.42
1:B:17:CYS:HA	1:B:308:ILE:HG13	2.02	0.42
1:B:39:ASN:HD21	1:B:42:GLU:HG3	1.85	0.41
1:D:345:ALA:C	1:D:347:GLU:N	2.73	0.41
1:A:80[B]:VAL:HB	1:A:234[B]:LEU:HD21	2.02	0.41
1:B:38:PRO:HB3	1:C:199:ILE:HD11	2.01	0.41
1:A:169:VAL:CG2	1:A:169:VAL:O	2.68	0.41
1:B:178:ARG:NE	5:X:2006:HOH:O	2.47	0.41
1:D:169:VAL:HA	1:D:170:PRO:HD3	1.96	0.41
1:D:203:ASN:ND2	1:D:206:GLU:HB2	2.35	0.41
2:Y:944:LYS:HA	2:Y:944:LYS:HD3	1.52	0.41
1:B:130:GLU:N	5:B:2074:HOH:O	2.12	0.41
1:A:164:GLU:HA	1:A:170:PRO:HA	2.02	0.41
1:A:296:GLU:HG3	1:A:301:ASN:N	2.35	0.41
1:A:166:LYS:C	1:A:168:ARG:HA	2.41	0.41
1:D:86:GLY:O	1:D:234[A]:LEU:HA	2.21	0.41
1:A:296:GLU:HG3	1:A:301:ASN:H	1.85	0.41
1:D:130:GLU:HA	2:W:949[B]:GLY:O	2.20	0.41
1:C:14:LYS:CE	5:C:2003:HOH:O	2.68	0.41
1:A:150:ARG:HH11	1:A:150:ARG:HD2	1.68	0.41
1:C:343:LEU:O	1:C:344:THR:HB	2.21	0.41
1:C:212:HIS:CE1	1:C:264:SER:OG	2.71	0.41
1:C:230:LEU:HD22	1:C:339:VAL:CG2	2.51	0.40
1:B:190:ILE:O	1:B:194:LYS:HG3	2.21	0.40
1:D:23:ASN:HD21	1:D:26:GLU:HG3	1.86	0.40
1:B:60:LYS:HB3	1:B:61:PRO:HD2	2.03	0.40
1:D:299:GLY:N	1:D:335:ASN:ND2	2.62	0.40
1:B:261:ILE:O	1:B:262:ASN:C	2.58	0.40
1:A:155[A]:VAL:HG11	1:A:199:ILE:CD1	2.51	0.40
1:A:234[A]:LEU:HD22	1:A:236:LEU:HG	2.04	0.40
1:D:73:ALA:O	1:D:76:ILE:HG22	2.22	0.40
1:C:348:TRP:HB2	1:D:348:TRP:CB	2.52	0.40
1:B:262:ASN:HD22	1:B:265:LEU:HG	1.87	0.40
1:B:286:ARG:HG2	1:B:292:ARG:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/365 (92%)	320 (96%)	11 (3%)	3 (1%)	21	19
1	B	343/365 (94%)	327 (95%)	15 (4%)	1 (0%)	46	50
1	C	342/365 (94%)	329 (96%)	7 (2%)	6 (2%)	11	7
1	D	340/365 (93%)	316 (93%)	20 (6%)	4 (1%)	16	12
2	W	21/20 (105%)	11 (52%)	6 (29%)	4 (19%)	0	0
2	X	11/20 (55%)	9 (82%)	2 (18%)	0	100	100
2	Y	10/20 (50%)	9 (90%)	1 (10%)	0	100	100
All	All	1401/1520 (92%)	1321 (94%)	62 (4%)	18 (1%)	16	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	9	ALA
1	C	260	ASN
1	C	344	THR
1	D	280	LYS
1	D	346	GLU
1	A	344	THR
1	A	169	VAL
1	C	49	ALA
1	C	130	GLU
2	W	948[A]	SER
2	W	948[B]	SER
1	A	131	VAL
1	D	244	LYS
2	W	940[A]	ALA
2	W	940[B]	ALA
1	B	75	SER
1	D	361	ARG
1	C	131	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/321 (91%)	273 (93%)	20 (7%)	20	21
1	B	297/321 (92%)	276 (93%)	21 (7%)	18	19
1	C	298/321 (93%)	281 (94%)	17 (6%)	25	29
1	D	295/321 (92%)	271 (92%)	24 (8%)	15	14
2	W	18/13 (138%)	14 (78%)	4 (22%)	1	1
2	X	9/13 (69%)	8 (89%)	1 (11%)	8	6
2	Y	9/13 (69%)	7 (78%)	2 (22%)	1	1
All	All	1219/1323 (92%)	1130 (93%)	89 (7%)	19	18

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	16	VAL
1	A	23	ASN
1	A	35	VAL
1	A	46	ILE
1	A	77[A]	VAL
1	A	77[B]	VAL
1	A	81	LEU
1	A	130	GLU
1	A	133	LEU
1	A	166	LYS
1	A	168	ARG
1	A	169	VAL
1	A	261	ILE
1	A	280	LYS
1	A	286	ARG
1	A	292	ARG
1	A	298	LEU
1	A	336	VAL
1	A	347	GLU

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Mol	Chain	Res	Type
1	B	22	LEU
1	B	23	ASN
1	B	35	VAL
1	B	46	ILE
1	B	47	SER
1	B	80	VAL
1	B	81	LEU
1	B	95	SER
1	B	133	LEU
1	B	166	LYS
1	B	169	VAL
1	B	170	PRO
1	B	236	LEU
1	B	244	LYS
1	B	263	LYS
1	B	264	SER
1	B	293[A]	ILE
1	B	293[B]	ILE
1	B	298	LEU
1	B	336	VAL
1	B	339	VAL
1	C	23	ASN
1	C	46[A]	ILE
1	C	46[B]	ILE
1	C	81	LEU
1	C	133	LEU
1	C	158	VAL
1	C	168	ARG
1	C	236	LEU
1	C	261	ILE
1	C	277	ASP
1	C	298	LEU
1	C	303	ARG
1	C	342	GLU
1	C	343	LEU
1	C	347	GLU
1	C	350	ARG
1	C	352	TYR
1	D	14	LYS
1	D	23	ASN
1	D	34	VAL
1	D	46	ILE

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Mol	Chain	Res	Type
1	D	47	SER
1	D	67	LYS
1	D	81	LEU
1	D	110	VAL
1	D	130	GLU
1	D	143	GLU
1	D	156	SER
1	D	173	LYS
1	D	231	SER
1	D	236	LEU
1	D	266	SER
1	D	287	ASP
1	D	296[A]	GLU
1	D	296[B]	GLU
1	D	298	LEU
1	D	318	SER
1	D	321	LYS
1	D	343	LEU
1	D	349	LYS
1	D	352	TYR
2	W	939[A]	GLN
2	W	939[B]	GLN
2	W	947[A]	ARG
2	W	947[B]	ARG
2	X	946	ILE
2	Y	944	LYS
2	Y	947	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	44	ASN
1	A	70	ASN
1	A	93	GLN
1	A	100	HIS
1	A	163	HIS
1	A	196	ASN
1	A	198	HIS
1	A	212	HIS
1	A	221	GLN
1	A	262	ASN

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Mol	Chain	Res	Type
1	A	316	ASN
1	A	335	ASN
1	A	340	ASN
1	B	23	ASN
1	B	70	ASN
1	B	93	GLN
1	B	100	HIS
1	B	112	GLN
1	B	125	HIS
1	B	167	ASN
1	B	198	HIS
1	B	212	HIS
1	B	221	GLN
1	B	262	ASN
1	B	316	ASN
1	B	335	ASN
1	B	340	ASN
1	C	23	ASN
1	C	70	ASN
1	C	93	GLN
1	C	100	HIS
1	C	112	GLN
1	C	125	HIS
1	C	196	ASN
1	C	212	HIS
1	C	221	GLN
1	C	279	ASN
1	C	295	GLN
1	C	316	ASN
1	C	335	ASN
1	C	340	ASN
1	D	23	ASN
1	D	70	ASN
1	D	93	GLN
1	D	100	HIS
1	D	112	GLN
1	D	125	HIS
1	D	196	ASN
1	D	203	ASN
1	D	205	ASN
1	D	207	HIS
1	D	212	HIS

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Mol	Chain	Res	Type
1	D	316	ASN
1	D	335	ASN
1	D	340	ASN
2	Y	941	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ADP	A	603	4	22,29,29	1.13	2 (9%)	27,45,45	1.85	6 (22%)
3	ADP	B	603	4	22,29,29	1.04	2 (9%)	27,45,45	2.21	7 (25%)
3	ADP	C	603	4	22,29,29	1.15	1 (4%)	27,45,45	2.18	7 (25%)
3	ADP	D	603	4	22,29,29	1.11	1 (4%)	27,45,45	2.16	7 (25%)

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	ADP	A	603	4	-	0/12/32/32	0/3/3/3
3	ADP	B	603	4	-	0/12/32/32	0/3/3/3
3	ADP	C	603	4	-	0/12/32/32	0/3/3/3
3	ADP	D	603	4	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	ADP	O4'-C1'	2.09	1.43	1.41
3	A	603	ADP	O4'-C1'	2.57	1.44	1.41
3	A	603	ADP	C5-C4	2.90	1.47	1.40
3	B	603	ADP	C5-C4	3.01	1.47	1.40
3	D	603	ADP	C5-C4	3.72	1.48	1.40
3	C	603	ADP	C5-C4	4.18	1.49	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	ADP	N3-C2-N1	-7.85	122.89	128.89
3	C	603	ADP	N3-C2-N1	-7.02	123.52	128.89
3	D	603	ADP	C2'-C1'-N9	-5.84	105.36	114.29
3	A	603	ADP	N3-C2-N1	-5.75	124.50	128.89
3	D	603	ADP	N3-C2-N1	-5.50	124.68	128.89
3	B	603	ADP	C4-C5-N7	-4.93	104.95	109.48
3	C	603	ADP	C4-C5-N7	-4.22	105.59	109.48
3	D	603	ADP	C4-C5-N7	-3.85	105.94	109.48
3	B	603	ADP	C2'-C1'-N9	-3.08	109.58	114.29
3	A	603	ADP	C4-C5-N7	-3.05	106.68	109.48
3	A	603	ADP	O3A-PA-O5'	-2.84	95.39	102.94
3	D	603	ADP	C1'-N9-C4	-2.75	122.80	126.94
3	A	603	ADP	C2'-C1'-N9	-2.74	110.11	114.29
3	C	603	ADP	C2'-C1'-N9	-2.67	110.21	114.29
3	A	603	ADP	O3'-C3'-C2'	-2.22	104.60	111.83
3	C	603	ADP	O3A-PA-O5'	-2.22	97.05	102.94
3	D	603	ADP	O3'-C3'-C2'	-2.10	105.00	111.83
3	D	603	ADP	PA-O3A-PB	-2.09	125.67	132.67
3	B	603	ADP	O4'-C1'-N9	-2.03	103.85	108.10
3	A	603	ADP	O3B-PB-O1B	2.05	117.17	110.58
3	B	603	ADP	O2B-PB-O1B	2.16	117.53	110.58
3	B	603	ADP	O2A-PA-O3A	2.33	115.67	105.09
3	B	603	ADP	O3B-PB-O2B	2.55	117.09	107.38
3	C	603	ADP	C2-N1-C6	2.60	123.41	118.77
3	D	603	ADP	C2-N1-C6	2.71	123.62	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	ADP	O3B-PB-O2B	2.90	118.44	107.38
3	C	603	ADP	C4'-O4'-C1'	4.27	114.42	109.72

There are no chirality outliers.

There are no torsion outliers.

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

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, 95th 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 ²)	Q<0.9
1	A	328/365 (89%)	0.10	21 (6%) 23 22	19, 32, 67, 99	0
1	B	341/365 (93%)	0.22	27 (7%) 15 15	21, 39, 70, 96	0
1	C	343/365 (93%)	0.19	35 (10%) 9 8	20, 36, 70, 91	0
1	D	338/365 (92%)	0.54	41 (12%) 6 5	31, 50, 83, 95	0
2	W	13/20 (65%)	0.77	2 (15%) 3 2	44, 49, 68, 74	3 (23%)
2	X	13/20 (65%)	1.36	3 (23%) 1 1	39, 44, 68, 69	13 (100%)
2	Y	12/20 (60%)	0.50	2 (16%) 2 2	28, 34, 46, 47	12 (100%)
All	All	1388/1520 (91%)	0.28	131 (9%) 11 10	19, 39, 75, 99	28 (2%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	938	PRO	9.2
1	D	352	TYR	8.9
1	C	8	PRO	8.9
1	D	281	THR	6.7
1	B	360	ALA	6.6
1	B	9	ALA	6.5
1	A	344	THR	5.6
1	D	279	ASN	5.4
1	D	278	GLY	5.3
1	C	49	ALA	4.8
1	D	360	ALA	4.8
1	D	166	LYS	4.5
1	A	281	THR	4.5
1	D	245	VAL	4.4
1	C	7	ILE	4.4
1	B	359	ASN	4.3
1	B	10	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	156	SER	4.2
1	B	363	LYS	4.1
1	A	8	PRO	4.1
1	A	350	ARG	4.1
1	D	277	ASP	3.9
1	B	245	VAL	3.9
1	A	351	ARG	3.8
1	B	237	VAL	3.8
2	W	949[B]	GLY	3.8
1	D	282	HIS	3.7
1	B	362	LEU	3.6
1	B	167	ASN	3.6
1	C	261	ILE	3.5
1	B	90	ALA	3.5
1	B	361	ARG	3.5
1	A	346	GLU	3.5
1	D	130	GLU	3.5
1	C	202	THR	3.5
1	A	237	VAL	3.4
1	D	132	ASN	3.4
1	D	336	VAL	3.4
1	D	351	ARG	3.4
1	C	158	VAL	3.4
1	C	237	VAL	3.4
1	D	361	ARG	3.3
1	C	9	ALA	3.3
1	D	236	LEU	3.3
2	W	938[A]	PRO	3.3
1	C	359	ASN	3.2
1	D	10	GLU	3.2
1	D	280	LYS	3.2
1	D	40	ASN	3.2
1	A	348	TRP	3.2
2	X	949	GLY	3.1
1	A	347	GLU	3.1
1	D	307	VAL	3.1
1	C	350	ARG	3.1
1	C	259	LYS	3.0
1	B	261	ILE	3.0
1	C	167	ASN	3.0
1	D	11	ASP	3.0
1	D	202	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	X	939	GLN	2.9
1	C	236	LEU	2.9
1	A	279	ASN	2.9
1	B	281	THR	2.9
1	C	352	TYR	2.9
1	A	307	VAL	2.8
1	A	236	LEU	2.8
1	C	356	LYS	2.8
1	D	90	ALA	2.8
1	B	358	LYS	2.7
1	D	237	VAL	2.7
1	C	200	ALA	2.7
1	C	214	VAL	2.7
1	D	155	VAL	2.7
1	D	127	TYR	2.6
1	C	166	LYS	2.6
1	C	309	CYS	2.5
1	C	306	ILE	2.5
1	B	279	ASN	2.5
1	A	155[A]	VAL	2.5
1	A	9	ALA	2.4
1	B	24	ASP	2.4
2	Y	949	GLY	2.4
1	C	88	ILE	2.4
1	D	350	ARG	2.4
1	B	89	PHE	2.4
1	A	343	LEU	2.4
1	B	308	ILE	2.4
1	D	49	ALA	2.4
1	D	244	LYS	2.4
1	C	353	GLU	2.3
1	C	131	VAL	2.3
1	C	307	VAL	2.3
1	B	236	LEU	2.3
1	D	239	LEU	2.3
1	A	167	ASN	2.3
1	B	307	VAL	2.3
1	D	214	VAL	2.3
1	C	360	ALA	2.3
1	A	234[A]	LEU	2.3
1	B	88	ILE	2.2
1	C	215	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	90	ALA	2.2
1	D	41	VAL	2.2
1	B	166	LYS	2.2
2	Y	939	GLN	2.2
1	A	315	PHE	2.2
1	B	165	ASP	2.2
1	C	168	ARG	2.2
1	D	306	ILE	2.1
1	C	348	TRP	2.1
1	D	210	ARG	2.1
1	D	356	LYS	2.1
1	A	99	THR	2.1
1	B	357	GLU	2.1
1	B	215	PHE	2.1
1	C	216	LEU	2.1
1	D	348	TRP	2.1
1	D	128	ALA	2.1
1	A	90	ALA	2.1
1	D	88	ILE	2.1
1	B	239	LEU	2.0
1	C	239	LEU	2.0
1	C	362	LEU	2.0
1	D	358	LYS	2.0
1	D	225	GLU	2.0
1	B	294[A]	LEU	2.0
1	D	359	ASN	2.0
1	A	349	LYS	2.0
1	C	87	THR	2.0
1	C	130	GLU	2.0
1	C	347	GLU	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, 95th 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 ²)	Q<0.9
3	ADP	B	603	27/27	0.98	0.10	-0.63	18,26,31,32	0
3	ADP	A	603	27/27	0.98	0.12	-0.86	14,23,28,30	0
3	ADP	C	603	27/27	0.98	0.10	-0.93	20,29,34,37	0
3	ADP	D	603	27/27	0.97	0.09	-1.09	29,35,39,44	0
4	MG	D	800	1/1	0.88	0.10	-	36,36,36,36	0
4	MG	A	800	1/1	0.99	0.22	-	20,20,20,20	0
4	MG	B	800	1/1	0.99	0.15	-	20,20,20,20	0
4	MG	C	800	1/1	0.91	0.10	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.