



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:17 AM GMT

PDB ID : 3A98
Title : Crystal structure of the complex of the interacting regions of DOCK2 and ELMO1
Authors : Hanawa-Suetsugu, K.; Kukimoto-Niino, M.; Sekine, S.; Ito, T.; Mishima-Tsumagari, C.; Terada, T.; Shirouzu, M.; Fukui, Y.; Yokoyama, S.
Deposited on : 2009-10-21
Resolution : 2.10 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

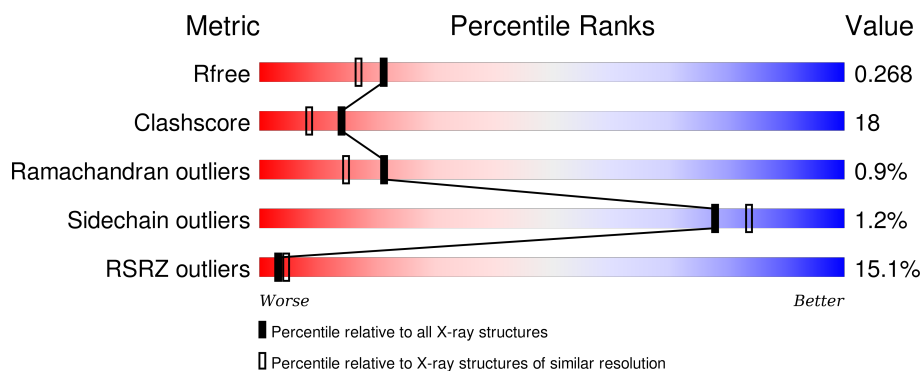
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	184	<div> <div>5%</div> <div>65%</div> <div>20%</div> <div>•</div> <div>15%</div> </div>
1	C	184	<div> <div>4%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>17%</div> </div>
2	B	203	<div> <div>14%</div> <div>64%</div> <div>29%</div> <div>•</div> <div>6%</div> </div>
2	D	203	<div> <div>26%</div> <div>49%</div> <div>33%</div> <div>•</div> <div>18%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5550 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 Dedicator of cytokinesis protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	Se	0	0	0
			1286	833	218	229	1	5			
1	C	152	Total	C	N	O	S	Se	0	0	0
			1243	804	210	223	1	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q92608
A	-5	SER	-	EXPRESSION TAG	UNP Q92608
A	-4	SER	-	EXPRESSION TAG	UNP Q92608
A	-3	GLY	-	EXPRESSION TAG	UNP Q92608
A	-2	SER	-	EXPRESSION TAG	UNP Q92608
A	-1	SER	-	EXPRESSION TAG	UNP Q92608
A	0	GLY	-	EXPRESSION TAG	UNP Q92608
C	-6	GLY	-	EXPRESSION TAG	UNP Q92608
C	-5	SER	-	EXPRESSION TAG	UNP Q92608
C	-4	SER	-	EXPRESSION TAG	UNP Q92608
C	-3	GLY	-	EXPRESSION TAG	UNP Q92608
C	-2	SER	-	EXPRESSION TAG	UNP Q92608
C	-1	SER	-	EXPRESSION TAG	UNP Q92608
C	0	GLY	-	EXPRESSION TAG	UNP Q92608

- Molecule 2 is a protein called Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	Se	0	0	0
			1539	975	262	292	6	4			
2	D	167	Total	C	N	O	S	Se	0	0	0
			1349	862	223	254	6	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	525	GLY	-	EXPRESSION TAG	UNP Q92556
B	526	SER	-	EXPRESSION TAG	UNP Q92556
B	527	SER	-	EXPRESSION TAG	UNP Q92556
B	528	GLY	-	EXPRESSION TAG	UNP Q92556
B	529	SER	-	EXPRESSION TAG	UNP Q92556
B	530	SER	-	EXPRESSION TAG	UNP Q92556
B	531	GLY	-	EXPRESSION TAG	UNP Q92556
D	525	GLY	-	EXPRESSION TAG	UNP Q92556
D	526	SER	-	EXPRESSION TAG	UNP Q92556
D	527	SER	-	EXPRESSION TAG	UNP Q92556
D	528	GLY	-	EXPRESSION TAG	UNP Q92556
D	529	SER	-	EXPRESSION TAG	UNP Q92556
D	530	SER	-	EXPRESSION TAG	UNP Q92556
D	531	GLY	-	EXPRESSION TAG	UNP Q92556

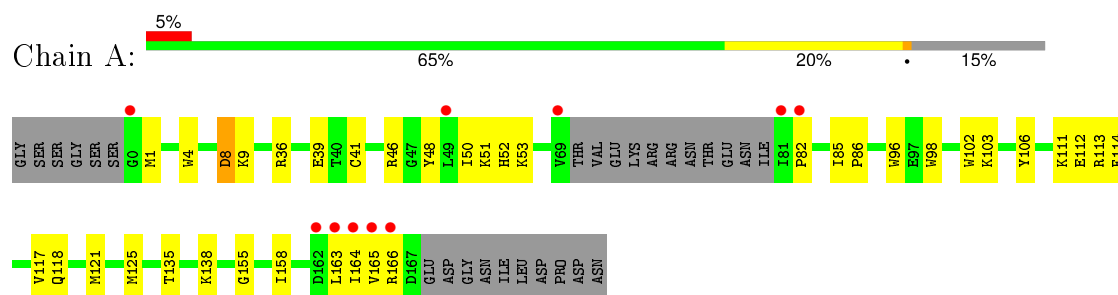
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	52	Total O 52 52	0	0
3	B	35	Total O 35 35	0	0
3	C	23	Total O 23 23	0	0
3	D	23	Total O 23 23	0	0

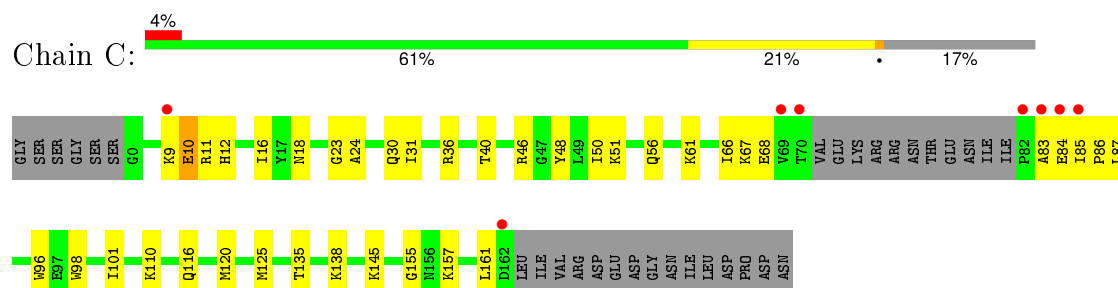
3 Residue-property plots [i](#)

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.

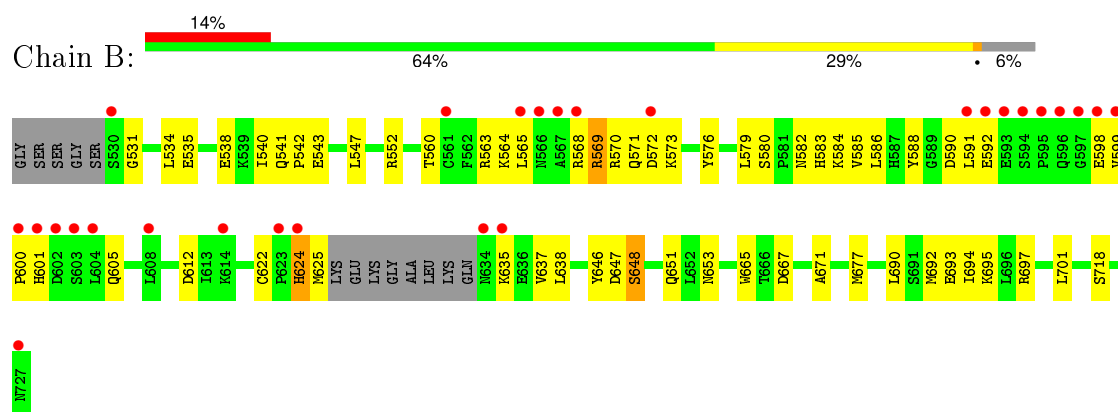
• Molecule 1: Dedicator of cytokinesis protein 2



• Molecule 1: Dedicator of cytokinesis protein 2

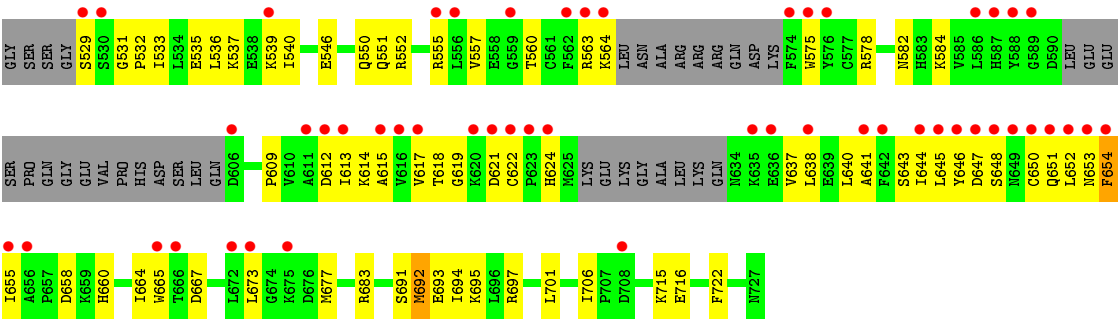


• Molecule 2: Engulfment and cell motility protein 1



• Molecule 2: Engulfment and cell motility protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.84Å 104.03Å 124.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 2.10 49.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.87-2.10) 99.6 (49.87-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.268 0.227 , 0.268	Depositor DCC
R_{free} test set	2455 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48976 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5550	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.41	0/1310	0.60	0/1757
1	C	0.40	0/1267	0.60	0/1698
2	B	0.33	0/1567	0.60	0/2114
2	D	0.30	0/1372	0.56	0/1848
All	All	0.36	0/5516	0.59	0/7417

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

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	1286	0	1314	39	0
1	C	1243	0	1263	40	0
2	B	1539	0	1534	66	0
2	D	1349	0	1348	75	0
3	A	52	0	0	0	0
3	B	35	0	0	0	0
3	C	23	0	0	0	0
3	D	23	0	0	3	0
All	All	5550	0	5459	199	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 18.

All (199) 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)
2:B:625:MSE:HE1	2:B:637:VAL:HG23	1.51	0.93
2:D:651:GLN:HE21	2:D:653:ASN:HD21	1.16	0.90
2:B:671:ALA:HB2	2:B:677:MSE:HE3	1.57	0.86
2:B:625:MSE:HE3	2:B:638:LEU:HD13	1.60	0.82
2:B:651:GLN:HE21	2:B:653:ASN:HD21	1.27	0.82
2:B:563:ARG:HH12	2:B:573:LYS:HB3	1.47	0.79
2:D:582:ASN:HD21	2:D:584:LYS:HB2	1.45	0.79
2:D:692:MSE:HA	2:D:692:MSE:CE	2.13	0.79
1:C:84:GLU:HG2	1:C:145:LYS:NZ	1.98	0.78
2:B:635:LYS:HA	2:B:638:LEU:HD23	1.65	0.78
2:D:692:MSE:HE3	2:D:692:MSE:HA	1.65	0.76
1:A:125:MSE:HE1	2:B:695:LYS:HD3	1.66	0.76
1:C:30:GLN:HE22	2:D:539:LYS:HG3	1.51	0.75
2:D:667:ASP:HB3	2:D:677:MSE:HE2	1.68	0.75
2:D:654:PHE:N	2:D:654:PHE:CD2	2.54	0.74
2:D:692:MSE:CE	2:D:695:LYS:HD2	2.18	0.74
2:D:552:ARG:HG3	2:D:677:MSE:HE1	1.70	0.74
1:A:82:PRO:HG2	1:A:85:ILE:HG12	1.70	0.74
1:A:125:MSE:HE1	2:B:695:LYS:CD	2.19	0.72
1:C:83:ALA:HB1	1:C:86:PRO:HG2	1.72	0.72
1:A:113:ARG:NH2	1:A:158:ILE:HB	2.04	0.71
2:B:622:CYS:HB3	2:B:624:HIS:CD2	2.25	0.71
2:B:625:MSE:HE2	2:B:638:LEU:HA	1.72	0.70
1:A:117:VAL:HG12	1:A:121:MSE:HE2	1.71	0.70
2:D:614:LYS:HG2	2:D:646:TYR:HA	1.72	0.70
2:B:543:GLU:O	2:B:547:LEU:HD13	1.90	0.70
2:D:651:GLN:HE21	2:D:653:ASN:ND2	1.87	0.69
2:B:563:ARG:NH1	2:B:573:LYS:HB3	2.07	0.69
1:A:125:MSE:HE1	2:B:695:LYS:HB3	1.75	0.68
2:B:579:LEU:HD11	2:B:583:HIS:HA	1.74	0.68
1:A:102:TRP:CD2	1:A:121:MSE:HE1	2.30	0.67
2:B:569:ARG:C	2:B:570:ARG:HG2	2.15	0.67
2:B:624:HIS:CD2	2:B:624:HIS:H	2.11	0.67
2:B:560:THR:HG21	2:B:665:TRP:HE1	1.60	0.67
2:D:654:PHE:HD2	2:D:654:PHE:N	1.92	0.66
1:C:36:ARG:HB2	1:C:50:ILE:HD11	1.76	0.66
1:C:85:ILE:HG23	1:C:86:PRO:HD3	1.77	0.66
1:C:84:GLU:HG2	1:C:145:LYS:HZ3	1.59	0.65
2:D:658:ASP:OD1	2:D:660:HIS:HB3	1.95	0.65
1:A:121:MSE:HE3	2:B:692:MSE:HE3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:575:TRP:HZ2	2:D:654:PHE:HB3	1.61	0.64
2:B:592:GLU:O	2:B:598:GLU:HA	1.96	0.64
2:D:582:ASN:ND2	2:D:584:LYS:HB2	2.13	0.64
2:D:715:LYS:HB3	2:D:715:LYS:NZ	2.12	0.64
2:D:529:SER:O	2:D:533:ILE:HD13	1.98	0.63
2:B:625:MSE:CE	2:B:638:LEU:HA	2.28	0.63
2:D:692:MSE:HE1	2:D:695:LYS:HD2	1.80	0.63
2:D:654:PHE:HD2	2:D:654:PHE:H	1.45	0.63
2:D:646:TYR:O	2:D:650:CYS:HB2	1.98	0.63
2:B:579:LEU:HD13	2:B:580:SER:O	1.98	0.63
2:B:560:THR:CG2	2:B:665:TRP:HE1	2.12	0.63
2:B:568:ARG:O	2:B:571:GLN:HG3	1.99	0.62
1:C:101:ILE:HD11	1:C:161:LEU:HD21	1.80	0.62
2:D:575:TRP:CZ2	2:D:654:PHE:HB3	2.33	0.62
2:D:552:ARG:HG3	2:D:677:MSE:CE	2.29	0.62
2:D:537:LYS:HG2	2:D:694:ILE:HD11	1.82	0.61
1:C:31:ILE:HD11	2:D:706:ILE:HD13	1.82	0.61
1:C:10:GLU:HB2	1:C:66:ILE:HD12	1.82	0.61
1:A:4:TRP:HA	1:A:41:CYS:HB2	1.83	0.61
2:B:624:HIS:HD2	2:B:624:HIS:H	1.49	0.61
1:C:85:ILE:N	1:C:86:PRO:HD2	2.16	0.60
2:D:613:ILE:HD12	2:D:644:ILE:CG2	2.31	0.60
2:D:667:ASP:CB	2:D:677:MSE:HE2	2.31	0.60
2:D:651:GLN:NE2	2:D:653:ASN:HD21	1.95	0.59
2:B:563:ARG:HH11	2:B:563:ARG:HG3	1.67	0.59
1:C:67:LYS:HG2	1:C:68:GLU:N	2.18	0.59
1:A:102:TRP:CE2	1:A:121:MSE:HE1	2.38	0.59
1:A:163:LEU:HD12	1:A:163:LEU:N	2.18	0.58
2:D:551:GLN:O	2:D:555:ARG:HG3	2.04	0.58
1:A:39:GLU:HG3	1:A:46:ARG:HB3	1.84	0.58
2:B:693:GLU:O	2:B:697:ARG:HG2	2.03	0.58
2:B:540:ILE:O	2:B:543:GLU:HG2	2.03	0.58
1:A:125:MSE:CE	2:B:695:LYS:HB3	2.34	0.58
1:A:1:MSE:HB2	2:B:718:SER:OG	2.05	0.57
2:B:565:LEU:HD23	2:B:565:LEU:H	1.69	0.57
2:D:640:LEU:HB2	2:D:655:ILE:HD11	1.87	0.57
2:B:564:LYS:NZ	2:B:590:ASP:OD1	2.36	0.56
2:D:622:CYS:HB3	2:D:624:HIS:NE2	2.21	0.56
2:D:697:ARG:HD3	3:D:35:HOH:O	2.05	0.56
1:A:135:THR:O	1:A:135:THR:HG22	2.05	0.56
2:B:569:ARG:O	2:B:570:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:ASN:ND2	2:B:584:LYS:HD2	2.20	0.55
2:B:651:GLN:NE2	2:B:653:ASN:HD21	2.00	0.55
1:C:18:ASN:HB3	3:D:13:HOH:O	2.07	0.55
1:C:83:ALA:O	1:C:87:LEU:HB2	2.08	0.54
2:B:625:MSE:CE	2:B:638:LEU:HD13	2.35	0.54
1:C:18:ASN:ND2	2:D:535:GLU:HG3	2.22	0.54
2:B:625:MSE:HE3	2:B:638:LEU:CD1	2.35	0.54
2:B:588:TYR:OH	2:B:605:GLN:HG2	2.07	0.54
1:C:85:ILE:N	1:C:86:PRO:CD	2.71	0.54
2:D:655:ILE:O	2:D:655:ILE:HG23	2.08	0.54
1:A:102:TRP:CG	1:A:121:MSE:HE1	2.43	0.54
1:A:113:ARG:HH21	1:A:158:ILE:HB	1.70	0.53
1:A:82:PRO:O	1:A:86:PRO:HD2	2.08	0.53
2:D:555:ARG:HD3	2:D:664:ILE:HD12	1.91	0.53
1:A:103:LYS:HD2	2:B:547:LEU:HD21	1.90	0.53
2:D:615:ALA:O	2:D:645:LEU:HB2	2.09	0.52
1:A:82:PRO:HG2	1:A:85:ILE:CG1	2.37	0.52
2:D:533:ILE:HD12	2:D:533:ILE:N	2.24	0.52
1:C:31:ILE:HG12	2:D:701:LEU:HD11	1.92	0.52
1:C:116:GLN:O	1:C:120:MSE:HG3	2.10	0.52
2:B:534:LEU:O	2:B:538:GLU:HG3	2.10	0.52
2:D:619:GLY:HA2	2:D:638:LEU:HD23	1.92	0.52
1:A:163:LEU:H	1:A:163:LEU:HD12	1.75	0.51
2:B:531:GLY:O	2:B:535:GLU:HG3	2.10	0.51
1:A:118:GLN:HA	1:A:121:MSE:HE3	1.93	0.51
1:A:51:LYS:NZ	1:A:96:TRP:NE1	2.54	0.51
2:D:624:HIS:HE1	2:D:641:ALA:HB1	1.75	0.51
2:D:715:LYS:HZ3	2:D:715:LYS:HB3	1.74	0.51
1:A:8:ASP:CG	1:A:9:LYS:H	2.15	0.51
2:D:613:ILE:HB	2:D:673:LEU:HD21	1.93	0.51
2:D:637:VAL:HG23	2:D:638:LEU:N	2.25	0.50
2:B:579:LEU:CD1	2:B:583:HIS:HA	2.39	0.50
2:D:529:SER:O	2:D:532:PRO:HD2	2.12	0.50
2:D:546:GLU:HG3	2:D:550:GLN:HE21	1.76	0.50
2:B:625:MSE:CE	2:B:638:LEU:HD22	2.41	0.49
1:C:30:GLN:HB3	2:D:536:LEU:HD13	1.94	0.49
1:A:118:GLN:HA	1:A:121:MSE:CE	2.41	0.49
1:C:31:ILE:HD11	2:D:706:ILE:CD1	2.42	0.49
1:A:121:MSE:CE	2:B:692:MSE:HE3	2.41	0.49
1:C:30:GLN:HE22	2:D:539:LYS:CG	2.23	0.49
2:D:613:ILE:HD12	2:D:644:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:624:HIS:CD2	2:D:643:SER:OG	2.66	0.49
2:B:625:MSE:HE3	2:B:638:LEU:HD22	1.93	0.49
1:C:40:THR:HG23	1:C:61:LYS:CE	2.43	0.49
1:C:10:GLU:O	1:C:10:GLU:HG2	2.13	0.48
2:D:617:VAL:CG2	2:D:643:SER:HB2	2.43	0.48
2:D:531:GLY:O	2:D:535:GLU:HG2	2.14	0.48
2:D:563:ARG:O	2:D:655:ILE:HG22	2.13	0.48
1:A:48:TYR:CE1	1:A:53:LYS:HG2	2.48	0.48
2:B:667:ASP:HB3	2:B:677:MSE:HE2	1.95	0.48
2:D:683:ARG:HB2	2:D:683:ARG:HE	1.51	0.48
2:B:572:ASP:OD2	2:B:601:HIS:HE1	1.97	0.47
2:D:640:LEU:C	2:D:655:ILE:HD12	2.34	0.47
1:A:36:ARG:HB2	1:A:50:ILE:HD11	1.95	0.47
1:A:121:MSE:O	1:A:125:MSE:HG3	2.14	0.47
2:B:563:ARG:NH1	2:B:563:ARG:HG3	2.29	0.47
2:D:564:LYS:HE3	2:D:575:TRP:CD1	2.49	0.47
2:B:591:LEU:CD2	2:B:600:PRO:HB3	2.45	0.47
1:A:125:MSE:HE1	2:B:695:LYS:CB	2.45	0.46
1:C:98:TRP:CZ2	1:C:155:GLY:HA3	2.51	0.46
1:C:84:GLU:N	1:C:86:PRO:HD2	2.31	0.46
2:D:624:HIS:CE1	2:D:641:ALA:HB1	2.50	0.46
1:A:106:TYR:HB2	1:A:114:PHE:CE1	2.50	0.46
2:B:622:CYS:HB2	2:B:625:MSE:HG2	1.97	0.46
2:D:647:ASP:HB2	2:D:650:CYS:SG	2.55	0.45
2:D:692:MSE:HE2	2:D:695:LYS:HB2	1.98	0.45
1:C:85:ILE:CG2	1:C:86:PRO:HD3	2.45	0.45
2:B:592:GLU:CG	2:B:599:VAL:HG23	2.47	0.45
1:C:11:ARG:HG2	1:C:12:HIS:CE1	2.52	0.45
1:C:125:MSE:SE	2:D:692:MSE:HE1	2.67	0.45
2:D:557:VAL:O	2:D:578:ARG:HG3	2.17	0.45
2:B:552:ARG:HB2	2:B:677:MSE:HE1	1.99	0.45
1:C:51:LYS:HE3	1:C:96:TRP:CE2	2.51	0.45
2:D:540:ILE:HG21	2:D:693:GLU:HG2	1.99	0.44
1:C:135:THR:HG22	1:C:135:THR:O	2.17	0.44
1:C:138:LYS:HD3	1:C:138:LYS:O	2.16	0.44
2:D:646:TYR:CE1	2:D:650:CYS:HB3	2.53	0.44
1:A:135:THR:O	1:A:135:THR:CG2	2.65	0.44
2:B:568:ARG:O	2:B:571:GLN:CG	2.65	0.44
2:D:560:THR:HG1	2:D:665:TRP:HE1	1.65	0.44
1:C:110:LYS:HA	1:C:110:LYS:HE2	2.00	0.44
2:D:693:GLU:O	2:D:697:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LYS:HG2	1:C:68:GLU:H	1.83	0.43
1:A:51:LYS:O	1:A:52:HIS:CG	2.70	0.43
2:D:618:THR:O	2:D:621:ASP:HB2	2.17	0.43
2:B:690:LEU:O	2:B:694:ILE:HG12	2.19	0.43
1:C:48:TYR:HB3	1:C:56:GLN:HB2	2.01	0.42
2:D:609:PRO:HB2	2:D:612:ASP:HB2	2.00	0.42
1:A:138:LYS:HB2	1:A:138:LYS:NZ	2.34	0.42
1:C:16:ILE:O	2:D:706:ILE:HG23	2.19	0.42
1:A:164:ILE:HG22	1:A:165:VAL:N	2.35	0.42
2:B:647:ASP:HB3	2:B:648:SER:H	1.62	0.42
1:C:23:GLY:O	1:C:24:ALA:C	2.58	0.42
2:D:646:TYR:HD1	2:D:647:ASP:OD2	2.03	0.42
2:B:591:LEU:HD23	2:B:600:PRO:CA	2.50	0.42
2:B:541:GLN:HB3	2:B:542:PRO:HD3	2.02	0.42
2:D:614:LYS:N	2:D:645:LEU:O	2.53	0.42
2:D:529:SER:HB2	3:D:94:HOH:O	2.19	0.42
1:A:96:TRP:HH2	2:B:697:ARG:HD3	1.85	0.41
2:D:624:HIS:HD2	2:D:643:SER:HG	1.67	0.41
1:C:157:LYS:HD3	1:C:157:LYS:O	2.19	0.41
2:B:601:HIS:ND1	2:B:601:HIS:O	2.52	0.41
2:D:691:SER:O	2:D:695:LYS:HG3	2.20	0.41
1:C:31:ILE:CD1	2:D:706:ILE:HD13	2.50	0.41
2:B:582:ASN:O	2:B:583:HIS:HB2	2.21	0.41
1:A:111:LYS:HG3	1:A:112:GLU:N	2.35	0.41
2:B:576:TYR:CD1	2:B:576:TYR:C	2.94	0.41
2:B:612:ASP:O	2:B:646:TYR:HB2	2.21	0.41
1:C:83:ALA:O	1:C:87:LEU:CB	2.69	0.41
2:B:565:LEU:H	2:B:565:LEU:CD2	2.31	0.41
2:D:622:CYS:HB3	2:D:624:HIS:CD2	2.56	0.41
2:B:585:VAL:HG12	2:B:586:LEU:N	2.34	0.41
1:A:98:TRP:CZ2	1:A:155:GLY:HA3	2.56	0.41
1:C:67:LYS:CG	1:C:68:GLU:N	2.82	0.41
2:B:591:LEU:HD21	2:B:600:PRO:HB3	2.03	0.40
2:B:582:ASN:HD21	2:B:584:LYS:HD2	1.84	0.40
1:C:46:ARG:HD2	2:D:722:PHE:CD1	2.57	0.40
1:A:8:ASP:N	1:A:8:ASP:OD2	2.54	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	153/184 (83%)	149 (97%)	2 (1%)	2 (1%)	15	9
1	C	148/184 (80%)	140 (95%)	7 (5%)	1 (1%)	26	21
2	B	186/203 (92%)	172 (92%)	12 (6%)	2 (1%)	17	11
2	D	159/203 (78%)	150 (94%)	8 (5%)	1 (1%)	30	24
All	All	646/774 (84%)	611 (95%)	29 (4%)	6 (1%)	21	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	648	SER
2	D	648	SER
1	A	166	ARG
1	C	9	LYS
1	A	8	ASP
2	B	569	ARG

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	139/158 (88%)	139 (100%)	0	100	100
1	C	134/158 (85%)	133 (99%)	1 (1%)	88	92
2	B	176/181 (97%)	174 (99%)	2 (1%)	80	85
2	D	155/181 (86%)	151 (97%)	4 (3%)	54	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	604/678 (89%)	597 (99%)	7 (1%)	78	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	624	HIS
2	B	701	LEU
1	C	10	GLU
2	D	652	LEU
2	D	654	PHE
2	D	692	MSE
2	D	716	GLU

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

Mol	Chain	Res	Type
2	B	554	ASN
2	B	566	ASN
2	B	583	HIS
2	B	624	HIS
2	B	649	ASN
2	B	651	GLN
2	B	703	ASN
1	C	30	GLN
1	C	130	GLN
1	C	146	GLN
2	D	550	GLN
2	D	624	HIS
2	D	649	ASN
2	D	651	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	152/184 (82%)	0.62	10 (6%)	22 29	25, 38, 80, 105	0
1	C	147/184 (79%)	0.62	8 (5%)	29 38	27, 40, 79, 104	0
2	B	186/203 (91%)	1.01	28 (15%)	3 4	27, 50, 98, 114	0
2	D	163/203 (80%)	1.61	52 (31%)	1 1	28, 65, 108, 124	0
All	All	648/774 (83%)	0.98	98 (15%)	3 4	25, 47, 102, 124	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	11.2
2	B	599	VAL	9.5
1	C	69	VAL	9.3
2	D	616	VAL	9.1
2	B	593	GLU	7.9
2	B	603	SER	7.4
2	D	564	LYS	7.2
2	D	615	ALA	7.0
2	D	623	PRO	6.7
2	B	597	GLY	6.5
2	B	594	SER	6.5
1	C	82	PRO	6.5
2	D	651	GLN	6.2
2	D	650	CYS	5.9
1	A	0	GLY	5.8
2	D	588	TYR	5.7
1	C	83	ALA	5.5
2	D	647	ASP	5.5
2	B	530	SER	5.4
2	B	600	PRO	5.4
2	D	613	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	642	PHE	5.3
2	D	622	CYS	5.1
2	B	568	ARG	5.1
2	D	646	TYR	5.1
2	B	595	PRO	4.9
2	D	612	ASP	4.8
2	D	644	ILE	4.8
2	B	604	LEU	4.7
2	D	576	TYR	4.7
2	D	574	PHE	4.7
2	B	566	ASN	4.6
2	D	563	ARG	4.6
2	B	602	ASP	4.4
2	D	655	ILE	4.4
2	D	638	LEU	4.4
2	D	673	LEU	4.3
2	D	649	ASN	4.2
1	C	70	THR	4.2
2	B	608	LEU	4.1
2	D	562	PHE	4.1
2	D	672	LEU	4.0
2	D	575	TRP	3.9
2	B	596	GLN	3.8
1	A	164	ILE	3.8
2	D	617	VAL	3.7
2	B	591	LEU	3.7
2	B	592	GLU	3.7
2	D	653	ASN	3.7
1	A	82	PRO	3.6
2	B	601	HIS	3.6
2	B	598	GLU	3.6
2	D	654	PHE	3.5
2	D	641	ALA	3.5
1	A	162	ASP	3.4
2	D	606	ASP	3.4
2	B	624	HIS	3.3
2	D	645	LEU	3.3
2	D	624	HIS	3.3
2	D	708	ASP	3.3
2	D	530	SER	3.2
2	B	727	ASN	3.1
2	D	556	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	656	ALA	3.0
1	A	166	ARG	3.0
2	D	611	ALA	3.0
2	D	586	LEU	2.9
2	B	565	LEU	2.9
1	A	165	VAL	2.9
2	D	635	LYS	2.8
1	C	9	LYS	2.8
2	B	561	CYS	2.8
2	D	620	LYS	2.8
1	A	69	VAL	2.8
1	C	84	GLU	2.7
2	B	634	ASN	2.7
2	D	665	TRP	2.6
2	D	648	SER	2.6
2	D	652	LEU	2.5
1	A	81	ILE	2.5
2	D	587	HIS	2.4
2	B	623	PRO	2.4
2	D	555	ARG	2.4
1	C	85	ILE	2.3
2	D	675	LYS	2.3
2	B	572	ASP	2.3
2	B	614	LYS	2.3
1	A	49	LEU	2.3
2	B	567	ALA	2.3
2	D	589	GLY	2.2
2	D	559	GLY	2.2
2	B	635	LYS	2.2
1	C	162	ASP	2.1
2	D	636	GLU	2.1
2	D	666	THR	2.1
2	D	621	ASP	2.1
2	D	539	LYS	2.1
2	D	529	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.