



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:28 AM GMT

PDB ID : 2QVA
Title : Crystal structure of Drosophila melanogaster Translin protein
Authors : Gupta, G.D.; Makde, R.D.; Kumar, V.
Deposited on : 2007-08-08
Resolution : 3.40 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

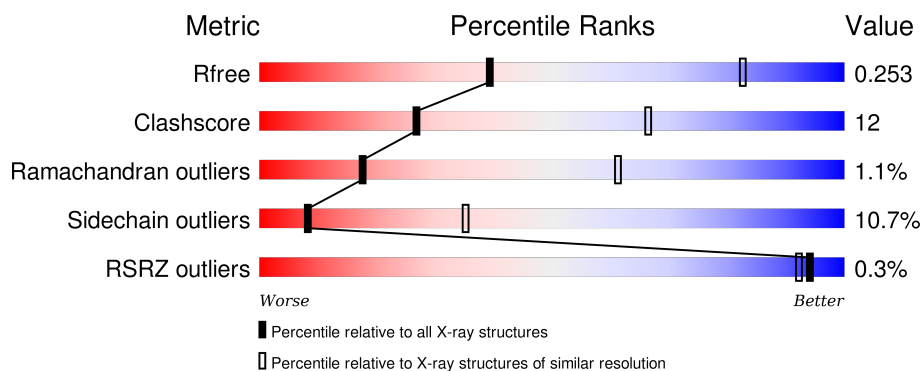
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	247	
1	B	247	
1	C	247	
1	D	247	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5925 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 GM27569p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1475	944	250	277	4			
1	B	182	Total	C	N	O	S	0	0	0
			1475	944	250	277	4			
1	C	185	Total	C	N	O	S	0	0	0
			1500	960	254	282	4			
1	D	182	Total	C	N	O	S	0	0	0
			1475	944	250	277	4			

There are 52 discrepancies between the modelled and reference sequences:

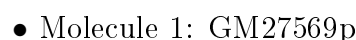
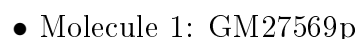
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q7JVK6
A	-10	ARG	-	EXPRESSION TAG	UNP Q7JVK6
A	-9	GLY	-	EXPRESSION TAG	UNP Q7JVK6
A	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
A	-7	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-6	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-5	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-4	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-3	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-2	HIS	-	EXPRESSION TAG	UNP Q7JVK6
A	-1	GLY	-	EXPRESSION TAG	UNP Q7JVK6
A	0	SER	-	EXPRESSION TAG	UNP Q7JVK6
A	168	SER	PRO	ENGINEERED	UNP Q7JVK6
B	-11	MET	-	EXPRESSION TAG	UNP Q7JVK6
B	-10	ARG	-	EXPRESSION TAG	UNP Q7JVK6
B	-9	GLY	-	EXPRESSION TAG	UNP Q7JVK6
B	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	-7	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-6	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-5	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-4	HIS	-	EXPRESSION TAG	UNP Q7JVK6

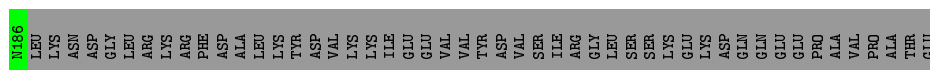
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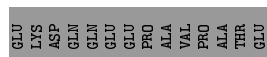
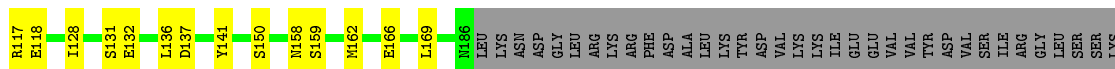
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-2	HIS	-	EXPRESSION TAG	UNP Q7JVK6
B	-1	GLY	-	EXPRESSION TAG	UNP Q7JVK6
B	0	SER	-	EXPRESSION TAG	UNP Q7JVK6
B	168	SER	PRO	ENGINEERED	UNP Q7JVK6
C	-11	MET	-	EXPRESSION TAG	UNP Q7JVK6
C	-10	ARG	-	EXPRESSION TAG	UNP Q7JVK6
C	-9	GLY	-	EXPRESSION TAG	UNP Q7JVK6
C	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
C	-7	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-6	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-5	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-4	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-3	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-2	HIS	-	EXPRESSION TAG	UNP Q7JVK6
C	-1	GLY	-	EXPRESSION TAG	UNP Q7JVK6
C	0	SER	-	EXPRESSION TAG	UNP Q7JVK6
C	168	SER	PRO	ENGINEERED	UNP Q7JVK6
D	-11	MET	-	EXPRESSION TAG	UNP Q7JVK6
D	-10	ARG	-	EXPRESSION TAG	UNP Q7JVK6
D	-9	GLY	-	EXPRESSION TAG	UNP Q7JVK6
D	-8	SER	-	EXPRESSION TAG	UNP Q7JVK6
D	-7	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-6	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-5	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-4	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-3	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-2	HIS	-	EXPRESSION TAG	UNP Q7JVK6
D	-1	GLY	-	EXPRESSION TAG	UNP Q7JVK6
D	0	SER	-	EXPRESSION TAG	UNP Q7JVK6
D	168	SER	PRO	ENGINEERED	UNP Q7JVK6

- Molecule 1: GM27569p





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4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.58Å 96.62Å 153.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 19.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.40) 91.0 (19.96-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.269 0.188 , 0.253	Depositor DCC
R_{free} test set	951 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.0	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 18803 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5925	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.76	1/1499 (0.1%)	0.80	1/2025 (0.0%)
1	B	0.75	0/1499	0.82	1/2025 (0.0%)
1	C	0.72	0/1525	0.80	1/2060 (0.0%)
1	D	0.70	0/1499	0.78	0/2025
All	All	0.73	1/6022 (0.0%)	0.80	3/8135 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	CYS	CB-SG	-6.50	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	115	VAL	CB-CA-C	-5.42	101.11	111.40
1	C	143	LEU	CA-CB-CG	-5.39	102.90	115.30

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	1475	0	1481	34	0
1	B	1475	0	1481	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1500	0	1501	43	0
1	D	1475	0	1481	29	0
All	All	5925	0	5944	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (144) 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:177:ASP:HB3	1:C:5:VAL:HG11	1.25	1.15
1:D:117:ARG:HH12	1:D:128:ILE:HG23	1.25	0.96
1:D:45:LEU:HD13	1:D:105:LEU:HD23	1.55	0.84
1:D:74:GLN:HA	1:D:74:GLN:OE1	1.77	0.84
1:B:37:LEU:HD12	1:B:69:CYS:HB3	1.60	0.83
1:B:14:GLN:O	1:B:18:ASP:HB2	1.79	0.83
1:C:14:GLN:O	1:C:18:ASP:HB2	1.81	0.80
1:D:117:ARG:NH1	1:D:128:ILE:HG23	1.96	0.80
1:A:100:ILE:HD13	1:A:141:TYR:HA	1.62	0.80
1:D:37:LEU:HD12	1:D:69:CYS:HB3	1.68	0.76
1:B:177:ASP:CB	1:C:5:VAL:HG11	2.11	0.76
1:A:5:VAL:HG22	1:A:5:VAL:O	1.86	0.76
1:B:51:ASP:OD2	1:B:54:GLN:HG2	1.87	0.75
1:B:104:ALA:HA	1:B:115:VAL:HG11	1.70	0.74
1:A:14:GLN:O	1:A:18:ASP:HB2	1.89	0.73
1:D:40:GLU:HG2	1:D:65:GLN:HE21	1.55	0.72
1:A:93:THR:HG23	1:A:97:GLN:HE21	1.55	0.70
1:C:37:LEU:HD12	1:C:69:CYS:HB3	1.74	0.69
1:A:93:THR:HG23	1:A:97:GLN:NE2	2.09	0.67
1:D:43:ILE:O	1:D:46:GLN:HB2	1.93	0.67
1:B:17:ILE:O	1:B:21:GLN:HG2	1.94	0.67
1:B:25:GLU:HA	1:B:25:GLU:OE1	1.96	0.66
1:C:35:GLU:HG2	1:C:95:ILE:HD11	1.77	0.65
1:D:71:GLN:O	1:D:74:GLN:HB2	1.97	0.65
1:C:74:GLN:OE1	1:C:74:GLN:HA	1.98	0.64
1:C:17:ILE:O	1:C:21:GLN:HG2	1.99	0.63
1:C:89:SER:HA	1:C:92:TRP:CZ2	2.35	0.61
1:B:104:ALA:HA	1:B:115:VAL:CG1	2.29	0.61
1:B:80:VAL:HG21	1:B:134:PHE:HE1	1.67	0.60
1:D:100:ILE:HD12	1:D:141:TYR:HA	1.84	0.59
1:C:180:THR:O	1:C:184:LEU:HD13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:SER:O	1:C:14:GLN:HG2	2.04	0.58
1:C:151:GLU:HA	1:C:154:ARG:NH1	2.18	0.58
1:A:25:GLU:HA	1:A:25:GLU:OE1	2.05	0.57
1:B:24:ARG:HG2	1:B:28:ARG:NH2	2.19	0.56
1:B:97:GLN:NE2	1:B:140:ASP:OD1	2.39	0.56
1:B:71:GLN:HA	1:B:74:GLN:HG2	1.88	0.55
1:D:40:GLU:HG2	1:D:65:GLN:NE2	2.20	0.55
1:D:24:ARG:HG2	1:D:28:ARG:HH22	1.72	0.54
1:B:119:THR:O	1:B:123:MET:HG3	2.08	0.54
1:D:118:GLU:HG3	1:D:128:ILE:HD11	1.90	0.54
1:B:100:ILE:HD11	1:B:136:LEU:HD11	1.91	0.53
1:B:11:SER:O	1:B:14:GLN:HG2	2.09	0.52
1:A:165:TYR:HD2	1:D:169:LEU:HD13	1.74	0.52
1:B:89:SER:HA	1:B:92:TRP:CZ2	2.45	0.52
1:B:86:TYR:CZ	1:C:87:ARG:HD2	2.46	0.52
1:A:106:VAL:O	1:A:110:GLU:HG3	2.10	0.52
1:A:17:ILE:O	1:A:21:GLN:HG2	2.09	0.51
1:C:5:VAL:O	1:C:5:VAL:HG13	2.11	0.51
1:C:103:ILE:HD13	1:C:120:VAL:HG13	1.92	0.50
1:D:24:ARG:NH1	1:D:91:HIS:HE1	2.10	0.50
1:A:74:GLN:OE1	1:A:74:GLN:HA	2.11	0.50
1:A:183:ARG:C	1:A:185:LEU:H	2.15	0.50
1:C:9:ILE:HA	1:C:12:ASN:ND2	2.27	0.50
1:D:24:ARG:HG2	1:D:28:ARG:NH2	2.27	0.49
1:C:151:GLU:HA	1:C:154:ARG:HH11	1.77	0.49
1:B:96:THR:O	1:B:100:ILE:HG12	2.12	0.49
1:A:100:ILE:HD11	1:A:136:LEU:HD11	1.94	0.49
1:A:151:GLU:HA	1:A:154:ARG:NH1	2.27	0.49
1:C:88:TYR:C	1:C:90:ASP:N	2.67	0.48
1:B:23:VAL:O	1:B:27:ILE:HG12	2.13	0.48
1:D:40:GLU:HG3	1:D:40:GLU:O	2.12	0.48
1:B:87:ARG:HD2	1:C:86:TYR:CZ	2.48	0.48
1:D:100:ILE:CD1	1:D:141:TYR:HA	2.44	0.48
1:A:104:ALA:HB1	1:A:148:LEU:HD22	1.95	0.48
1:B:5:VAL:CG1	1:C:177:ASP:HB3	2.44	0.48
1:B:18:ASP:O	1:B:21:GLN:HB2	2.14	0.48
1:B:124:LEU:HB2	1:B:126:LEU:HD12	1.96	0.48
1:C:158:ASN:O	1:C:162:MET:HE2	2.14	0.48
1:C:184:LEU:C	1:C:185:LEU:HD12	2.33	0.48
1:B:117:ARG:HH12	1:B:128:ILE:HG23	1.78	0.48
1:A:102:ILE:O	1:A:106:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASN:HB3	1:A:8:ASP:HB2	1.96	0.47
1:C:119:THR:O	1:C:122:GLU:HB2	2.14	0.47
1:C:55:ILE:O	1:C:59:CYS:HB2	2.14	0.47
1:A:117:ARG:HG3	1:A:136:LEU:HD23	1.97	0.47
1:A:40:GLU:OE1	1:A:65:GLN:NE2	2.47	0.47
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.67	0.47
1:D:43:ILE:HA	1:D:43:ILE:HD12	1.84	0.47
1:D:39:LYS:O	1:D:43:ILE:HB	2.15	0.46
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.71	0.46
1:B:99:LEU:HA	1:B:99:LEU:HD23	1.54	0.46
1:A:163:GLY:HA2	1:A:165:TYR:CE1	2.51	0.46
1:C:88:TYR:C	1:C:90:ASP:H	2.18	0.46
1:B:43:ILE:HD12	1:B:43:ILE:HA	1.91	0.46
1:B:109:LEU:HA	1:B:109:LEU:HD23	1.65	0.46
1:C:88:TYR:O	1:C:90:ASP:N	2.49	0.46
1:B:6:ASN:OD1	1:B:8:ASP:HB2	2.16	0.45
1:B:65:GLN:NE2	1:B:65:GLN:HA	2.31	0.45
1:D:118:GLU:HG3	1:D:128:ILE:CD1	2.45	0.45
1:B:150:SER:O	1:B:153:SER:HB3	2.16	0.45
1:C:116:THR:O	1:C:120:VAL:HG23	2.17	0.45
1:C:126:LEU:HD12	1:C:136:LEU:HB2	1.98	0.45
1:C:89:SER:HA	1:C:92:TRP:CE2	2.52	0.44
1:D:69:CYS:O	1:D:73:TYR:HD1	2.00	0.44
1:D:41:ALA:HB2	1:D:65:GLN:HG3	1.98	0.44
1:C:80:VAL:HA	1:C:81:PRO:HD3	1.81	0.44
1:D:99:LEU:HA	1:D:99:LEU:HD23	1.89	0.44
1:C:116:THR:HB	1:C:118:GLU:OE1	2.18	0.44
1:A:89:SER:HA	1:A:92:TRP:CZ2	2.52	0.44
1:B:25:GLU:OE1	1:B:28:ARG:NH1	2.50	0.44
1:A:5:VAL:O	1:A:5:VAL:CG2	2.58	0.44
1:C:35:GLU:HG2	1:C:95:ILE:CD1	2.46	0.44
1:A:75:LYS:O	1:A:78:GLU:HG2	2.16	0.44
1:D:40:GLU:O	1:D:44:LYS:HG2	2.18	0.43
1:B:117:ARG:HA	1:B:120:VAL:HG23	1.99	0.43
1:A:38:SER:HB3	1:A:98:ARG:HH21	1.83	0.43
1:A:45:LEU:HD23	1:A:58:ALA:HB1	2.01	0.43
1:A:59:CYS:O	1:A:63:ARG:HB2	2.18	0.43
1:B:5:VAL:HG11	1:C:177:ASP:HB3	1.99	0.43
1:B:114:LEU:HD11	1:B:145:ILE:HD12	2.01	0.43
1:B:103:ILE:HD13	1:B:120:VAL:HG12	2.00	0.43
1:A:88:TYR:O	1:A:90:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ILE:HD13	1:D:95:ILE:HA	1.63	0.43
1:C:82:ALA:HB3	1:C:84:GLN:HE21	1.84	0.43
1:B:45:LEU:O	1:B:48:ILE:HG12	2.18	0.43
1:D:24:ARG:HH11	1:D:91:HIS:HE1	1.65	0.42
1:C:168:SER:HA	1:C:171:ILE:HD12	2.00	0.42
1:D:65:GLN:HA	1:D:65:GLN:OE1	2.19	0.42
1:C:146:LEU:HD12	1:C:182:PHE:CZ	2.55	0.42
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.69	0.42
1:B:102:ILE:O	1:B:103:ILE:C	2.57	0.42
1:B:146:LEU:HD13	1:B:182:PHE:CE2	2.55	0.42
1:C:99:LEU:HA	1:C:99:LEU:HD23	1.63	0.42
1:A:28:ARG:HE	1:A:28:ARG:HB2	1.68	0.42
1:C:9:ILE:HA	1:C:12:ASN:HD21	1.85	0.42
1:A:145:ILE:O	1:A:148:LEU:HB3	2.20	0.42
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.86	0.42
1:B:11:SER:HA	1:B:14:GLN:HE21	1.84	0.42
1:A:183:ARG:C	1:A:185:LEU:N	2.73	0.42
1:A:156:ALA:HA	1:A:171:ILE:HD12	2.01	0.42
1:B:95:ILE:HA	1:B:95:ILE:HD13	1.71	0.41
1:D:132:GLU:HG3	1:D:132:GLU:H	1.63	0.41
1:C:55:ILE:HG23	1:C:109:LEU:HD13	2.02	0.41
1:B:117:ARG:NH1	1:B:128:ILE:HG23	2.34	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.81	0.41
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.76	0.41
1:C:37:LEU:CD1	1:C:69:CYS:HB3	2.47	0.41
1:C:33:GLU:O	1:C:37:LEU:HG	2.21	0.40
1:B:48:ILE:HD12	1:B:155:PHE:CD1	2.55	0.40
1:C:43:ILE:O	1:C:46:GLN:HB2	2.21	0.40
1:C:109:LEU:HA	1:C:109:LEU:HD23	1.87	0.40
1:D:158:ASN:O	1:D:162:MET:HE2	2.20	0.40
1:A:108:TYR:CD2	1:A:108:TYR:C	2.94	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	180/247 (73%)	162 (90%)	15 (8%)	3 (2%)	11	51
1	B	180/247 (73%)	163 (91%)	16 (9%)	1 (1%)	30	72
1	C	183/247 (74%)	163 (89%)	17 (9%)	3 (2%)	12	53
1	D	180/247 (73%)	163 (91%)	16 (9%)	1 (1%)	30	72
All	All	723/988 (73%)	651 (90%)	64 (9%)	8 (1%)	17	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	LEU
1	A	130	GLN
1	A	131	SER
1	B	184	LEU
1	C	184	LEU
1	D	131	SER
1	C	130	GLN
1	C	132	GLU

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	161/219 (74%)	142 (88%)	19 (12%)	6	29
1	B	161/219 (74%)	139 (86%)	22 (14%)	4	23
1	C	164/219 (75%)	149 (91%)	15 (9%)	12	44
1	D	161/219 (74%)	148 (92%)	13 (8%)	15	51
All	All	647/876 (74%)	578 (89%)	69 (11%)	8	35

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	ILE
1	A	11	SER
1	A	12	ASN
1	A	14	GLN
1	A	17	ILE
1	A	19	ASN
1	A	38	SER
1	A	43	ILE
1	A	47	ILE
1	A	61	LEU
1	A	63	ARG
1	A	87	ARG
1	A	93	THR
1	A	115	VAL
1	A	132	GLU
1	A	150	SER
1	A	153	SER
1	A	185	LEU
1	B	9	ILE
1	B	16	TYR
1	B	17	ILE
1	B	59	CYS
1	B	63	ARG
1	B	68	LEU
1	B	90	ASP
1	B	93	THR
1	B	95	ILE
1	B	115	VAL
1	B	120	VAL
1	B	131	SER
1	B	137	ASP
1	B	146	LEU
1	B	150	SER
1	B	154	ARG
1	B	161	THR
1	B	166	GLU
1	B	173	HIS
1	B	175	ILE
1	B	180	THR
1	B	186	ASN
1	C	12	ASN
1	C	17	ILE

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Mol	Chain	Res	Type
1	C	26	ASN
1	C	38	SER
1	C	43	ILE
1	C	47	ILE
1	C	50	SER
1	C	90	ASP
1	C	93	THR
1	C	115	VAL
1	C	116	THR
1	C	131	SER
1	C	153	SER
1	C	172	SER
1	C	183	ARG
1	D	14	GLN
1	D	17	ILE
1	D	18	ASP
1	D	22	GLU
1	D	40	GLU
1	D	43	ILE
1	D	61	LEU
1	D	95	ILE
1	D	136	LEU
1	D	137	ASP
1	D	150	SER
1	D	159	SER
1	D	166	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	158	ASN
1	B	14	GLN
1	B	54	GLN
1	B	65	GLN
1	B	158	ASN
1	B	186	ASN
1	C	12	ASN
1	C	84	GLN
1	C	130	GLN
1	C	147	GLN
1	C	158	ASN

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Mol	Chain	Res	Type
1	C	179	ASN
1	D	91	HIS
1	D	158	ASN

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](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	182/247 (73%)	-0.58	0 100 100	18, 40, 60, 68	0
1	B	182/247 (73%)	-0.61	0 100 100	19, 42, 61, 68	0
1	C	185/247 (74%)	-0.63	2 (1%) 82 77	18, 41, 62, 80	0
1	D	182/247 (73%)	-0.55	0 100 100	17, 40, 61, 69	0
All	All	731/988 (73%)	-0.59	2 (0%) 94 92	17, 41, 62, 80	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	SER	3.8
1	C	132	GLU	3.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.