



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:57 AM UTC

PDB ID : 2QVA / pdb_00002qva
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

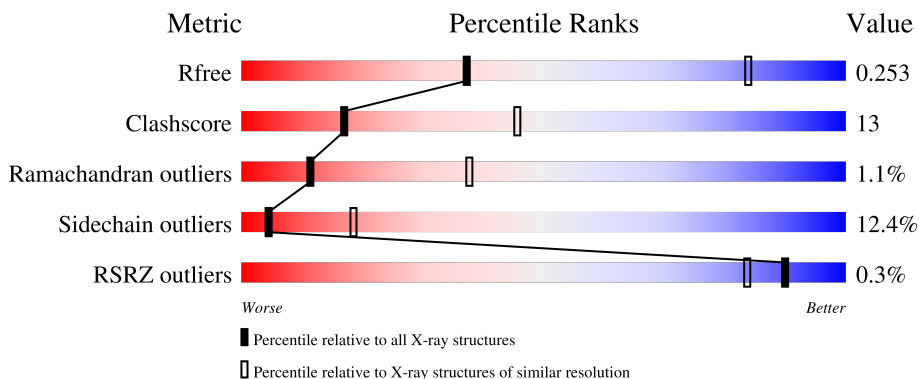
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	44% 26% • 26%
1	B	247	42% 27% • 26%
1	C	247	47% 26% • 25%
1	D	247	57% 15% • 26%

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 mutation	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

Continued on next page...

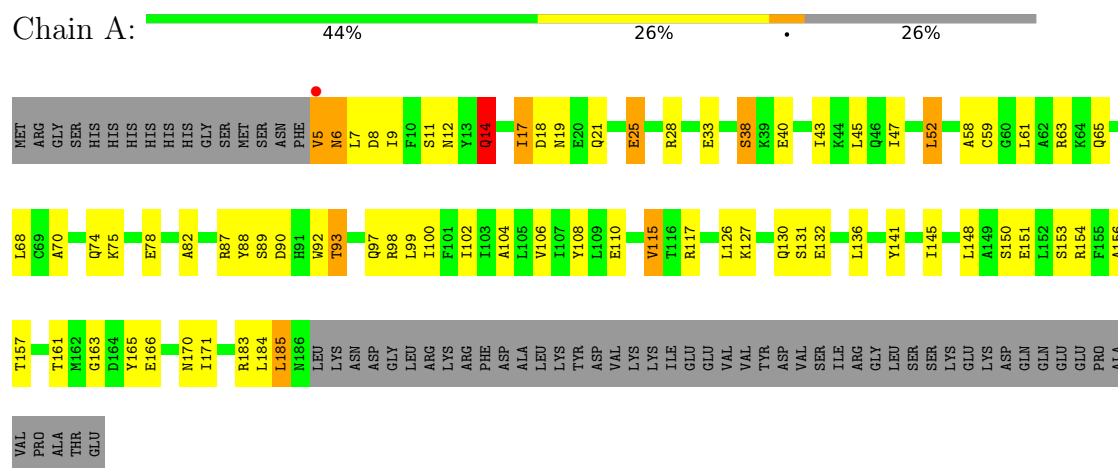
Continued from previous page...

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 mutation	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 mutation	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 mutation	UNP Q7JVK6

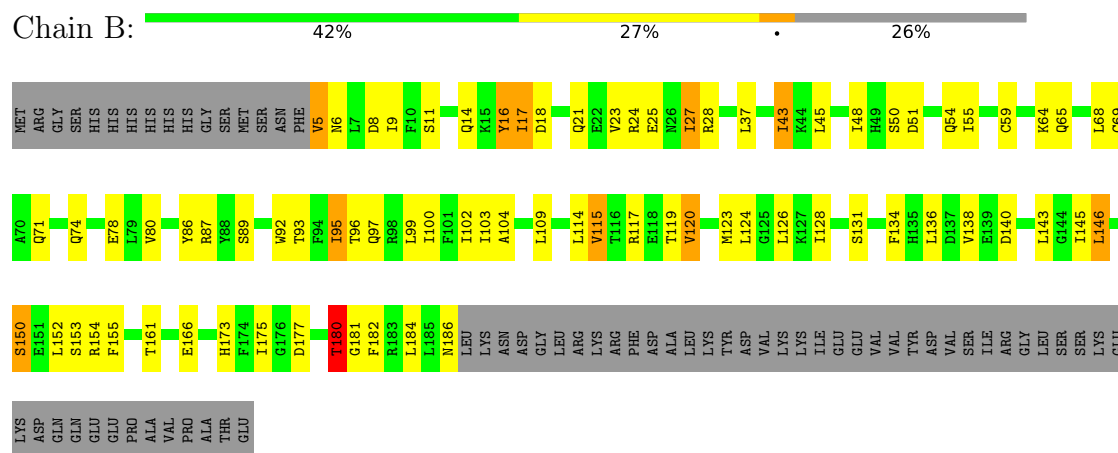
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

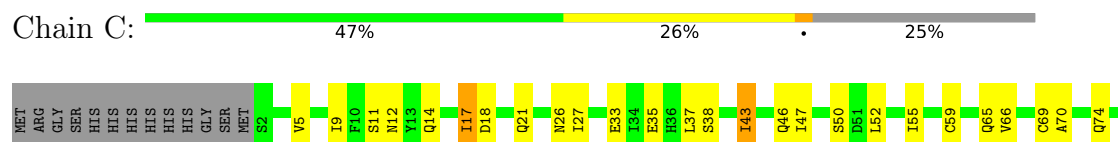
• Molecule 1: GM27569p

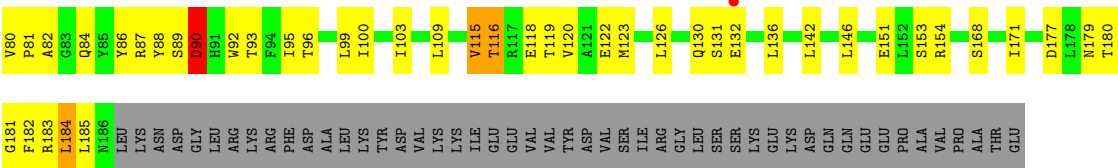


• Molecule 1: GM27569p



• Molecule 1: GM27569p





● Molecule 1: GM27569p



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 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.40) 90.4 (20.00-3.40)	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 (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.91	0/1499	1.09	5/2025 (0.2%)
1	B	0.89	0/1499	1.19	4/2025 (0.2%)
1	C	0.83	0/1525	1.11	5/2060 (0.2%)
1	D	0.88	0/1499	1.10	3/2025 (0.1%)
All	All	0.88	0/6022	1.12	17/8135 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	ALA	N-CA-C	-8.63	101.36	112.23
1	C	90	ASP	N-CA-C	7.02	119.01	111.36
1	A	115	VAL	CB-CA-C	-6.68	101.11	111.26
1	B	138	VAL	N-CA-C	6.66	117.16	110.23
1	B	27	ILE	N-CA-C	-6.23	104.44	110.42
1	D	115	VAL	CB-CA-C	-6.07	102.15	111.08
1	A	70	ALA	N-CA-C	-5.56	105.37	111.82
1	B	55	ILE	CB-CA-C	-5.52	104.91	111.81
1	D	70	ALA	N-CA-C	-5.50	105.29	112.23
1	C	115	VAL	CB-CA-C	-5.34	103.22	111.08
1	D	106	VAL	N-CA-C	5.34	115.78	110.23
1	C	100	ILE	CB-CA-C	-5.33	105.06	112.04
1	A	6	ASN	N-CA-C	5.25	118.18	109.46
1	A	82	ALA	CB-CA-C	-5.21	110.55	116.54
1	C	52	LEU	N-CA-C	5.16	119.06	112.87
1	B	180	THR	N-CA-C	-5.06	105.66	111.07
1	A	14	GLN	CA-CB-CG	5.01	124.11	114.10

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	1475	0	1481	36	0
1	B	1475	0	1481	47	0
1	C	1500	0	1501	45	0
1	D	1475	0	1481	30	0
All	All	5925	0	5944	151	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 13.

All (151) 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:14:GLN:O	1:B:18:ASP:HB2	1.79	0.83
1:B:37:LEU:HD12	1:B:69:CYS:HB3	1.60	0.83
1:C:14:GLN:O	1:C:18:ASP:HB2	1.81	0.80
1:A:100:ILE:HD13	1:A:141:TYR:HA	1.62	0.80
1:D:117:ARG:NH1	1:D:128:ILE:HG23	1.96	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:O	1:A:5:VAL:HG22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:GLN:O	1:D:74:GLN:HB2	1.97	0.65
1:C:74:GLN:HA	1:C:74:GLN:OE1	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
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:OE1	1:A:25:GLU:HA	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:A:183:ARG:C	1:A:185:LEU:H	2.15	0.54
1:B:119:THR:O	1:B:123:MET:HG3	2.08	0.54
1:D:24:ARG:HG2	1:D:28:ARG:HH22	1.72	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:C:184:LEU:C	1:C:185:LEU:HD12	2.33	0.52
1:A:165:TYR:HD2	1:D:169:LEU:HD13	1.74	0.52
1:A:106:VAL:O	1:A:110:GLU:HG3	2.10	0.52
1:B:86:TYR:CZ	1:C:87:ARG:HD2	2.46	0.52
1:B:89:SER:HA	1:B:92:TRP:CZ2	2.45	0.52
1:A:17:ILE:O	1:A:21:GLN:HG2	2.09	0.51
1:C:5:VAL:HG13	1:C:5:VAL:O	2.11	0.51
1:C:88:TYR:C	1:C:90:ASP:H	2.18	0.51
1:C:103:ILE:HD13	1:C:120:VAL:HG13	1.92	0.50
1:A:74:GLN:OE1	1:A:74:GLN:HA	2.11	0.50
1:C:88:TYR:C	1:C:90:ASP:N	2.67	0.50
1:D:24:ARG:NH1	1:D:91:HIS:HE1	2.10	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:B:23:VAL:O	1:B:27:ILE:HG12	2.13	0.48
1:B:87:ARG:HD2	1:C:86:TYR:CZ	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:GLU:O	1:D:40:GLU:HG3	2.12	0.48
1:A:104:ALA:HB1	1:A:148:LEU:HD22	1.95	0.48
1:D:100:ILE:CD1	1:D:141:TYR:HA	2.44	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: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
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:40:GLU:OE1	1:A:65:GLN:NE2	2.47	0.47
1:A:117:ARG:HG3	1:A:136:LEU:HD23	1.97	0.47
1:B:102:ILE:O	1:B:103:ILE:C	2.57	0.47
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.67	0.47
1:A:183:ARG:C	1:A:185:LEU:N	2.73	0.47
1:D:43:ILE:HD12	1:D:43:ILE:HA	1.84	0.47
1:D:39:LYS:O	1:D:43:ILE:HB	2.15	0.46
1:B:152:LEU:HD23	1:B:152:LEU:HA	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:B:43:ILE:HD12	1:B:43:ILE:HA	1.91	0.46
1:B:109:LEU:HD23	1:B:109:LEU:HA	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:A:108:TYR:CD2	1:A:108:TYR:C	2.94	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:C:65:GLN:O	1:C:66:VAL:C	2.59	0.44
1:C:80:VAL:HA	1:C:81:PRO:HD3	1.81	0.44
1:D:41:ALA:HB2	1:D:65:GLN:HG3	1.98	0.44
1:D:69:CYS:O	1:D:73:TYR:HD1	2.00	0.44
1:D:99:LEU:O	1:D:100:ILE:C	2.60	0.44
1:D:99:LEU:HD23	1:D:99:LEU:HA	1.89	0.44
1:A:89:SER:HA	1:A:92:TRP:CZ2	2.52	0.44
1:C:116:THR:HB	1:C:118:GLU:OE1	2.18	0.44
1:B:25:GLU:OE1	1:B:28:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:O	1:A:5:VAL:CG2	2.58	0.44
1:A:75:LYS:O	1:A:78:GLU:HG2	2.16	0.44
1:C:35:GLU:HG2	1:C:95:ILE:CD1	2.46	0.44
1:D:40:GLU:O	1:D:44:LYS:HG2	2.18	0.43
1:A:38:SER:HB3	1:A:98:ARG:HH21	1.83	0.43
1:B:117:ARG:HA	1:B:120:VAL:HG23	1.99	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:A:88:TYR:O	1:A:90:ASP:N	2.51	0.43
1:B:103:ILE:HD13	1:B:120:VAL:HG12	2.00	0.43
1:D:95:ILE:HD13	1:D:95:ILE:HA	1.63	0.43
1:B:45:LEU:O	1:B:48:ILE:HG12	2.18	0.43
1:B:180:THR:O	1:B:181:GLY:C	2.62	0.43
1:C:82:ALA:HB3	1:C:84:GLN:HE21	1.84	0.43
1:C:168:SER:HA	1:C:171:ILE:HD12	2.00	0.42
1:D:24:ARG:HH11	1:D:91:HIS:HE1	1.65	0.42
1:A:99:LEU:HA	1:A:99:LEU:HD23	1.69	0.42
1:C:123:MET:HE2	1:C:123:MET:HB3	1.85	0.42
1:C:146:LEU:HD12	1:C:182:PHE:CZ	2.55	0.42
1:D:65:GLN:HA	1:D:65:GLN:OE1	2.19	0.42
1:A:28:ARG:HE	1:A:28:ARG:HB2	1.68	0.42
1:A:170:ASN:O	1:A:171:ILE:C	2.63	0.42
1:B:146:LEU:HD13	1:B:182:PHE:CE2	2.55	0.42
1:C:99:LEU:HD23	1:C:99:LEU:HA	1.63	0.42
1:A:145:ILE:O	1:A:148:LEU:HB3	2.20	0.42
1:C:9:ILE:HA	1:C:12:ASN:HD21	1.85	0.42
1:B:16:TYR:CD2	1:B:16:TYR:C	2.97	0.42
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.86	0.42
1:A:156:ALA:HA	1:A:171:ILE:HD12	2.01	0.42
1:B:11:SER:HA	1:B:14:GLN:HE21	1.84	0.42
1:B:95:ILE:HD13	1:B:95:ILE:HA	1.71	0.41
1:C:179:ASN:C	1:C:181:GLY:N	2.76	0.41
1:D:132:GLU:H	1:D:132:GLU:HG3	1.63	0.41
1:C:55:ILE:HG23	1:C:109:LEU:HD13	2.02	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:B:117:ARG:NH1	1:B:128:ILE:HG23	2.34	0.41
1:D:162:MET:HE3	1:D:162:MET:HB2	1.89	0.41
1:A:126:LEU:C	1:A:127:LYS:HD3	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:CD1	1:C:69:CYS:HB3	2.47	0.41
1:B:48:ILE:HD12	1:B:155:PHE:CD1	2.55	0.40
1:C:33:GLU:O	1:C:37:LEU:HG	2.21	0.40
1:C:43:ILE:O	1:C:46:GLN:HB2	2.21	0.40
1:C:109:LEU:HD23	1:C:109:LEU:HA	1.87	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	180/247 (73%)	162 (90%)	15 (8%)	3 (2%)	7	28
1	B	180/247 (73%)	163 (91%)	16 (9%)	1 (1%)	21	50
1	C	183/247 (74%)	163 (89%)	17 (9%)	3 (2%)	7	29
1	D	180/247 (73%)	163 (91%)	16 (9%)	1 (1%)	21	50
All	All	723/988 (73%)	651 (90%)	64 (9%)	8 (1%)	11	38

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%)	135 (84%)	26 (16%)	2	10
1	B	161/219 (74%)	137 (85%)	24 (15%)	3	12
1	C	164/219 (75%)	149 (91%)	15 (9%)	9	30
1	D	161/219 (74%)	146 (91%)	15 (9%)	8	29
All	All	647/876 (74%)	567 (88%)	80 (12%)	4	18

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
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	25	GLU
1	A	33	GLU
1	A	38	SER
1	A	43	ILE
1	A	47	ILE
1	A	52	LEU
1	A	61	LEU
1	A	68	LEU
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	157	THR
1	A	161	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	166	GLU
1	A	185	LEU
1	B	5	VAL
1	B	9	ILE
1	B	16	TYR
1	B	17	ILE
1	B	43	ILE
1	B	50	SER
1	B	59	CYS
1	B	64	LYS
1	B	68	LEU
1	B	78	GLU
1	B	93	THR
1	B	95	ILE
1	B	115	VAL
1	B	120	VAL
1	B	131	SER
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	17	ILE
1	C	26	ASN
1	C	27	ILE
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	96	THR
1	C	115	VAL
1	C	116	THR
1	C	131	SER
1	C	153	SER
1	C	183	ARG
1	D	14	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	93	THR
1	D	95	ILE
1	D	100	ILE
1	D	136	LEU
1	D	137	ASP
1	D	150	SER
1	D	159	SER
1	D	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	147	GLN
1	A	158	ASN
1	A	173	HIS
1	B	14	GLN
1	B	54	GLN
1	B	65	GLN
1	B	91	HIS
1	B	158	ASN
1	B	186	ASN
1	C	12	ASN
1	C	84	GLN
1	C	147	GLN
1	C	158	ASN
1	C	179	ASN
1	C	186	ASN
1	D	6	ASN
1	D	46	GLN
1	D	91	HIS
1	D	97	GLN
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 oligosaccharides 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%)	-0.61	1 (0%) 87 78	18, 40, 60, 68	0
1	B	182/247 (73%)	-0.63	0 100 100	19, 42, 61, 68	0
1	C	185/247 (74%)	-0.61	1 (0%) 87 78	18, 41, 62, 80	0
1	D	182/247 (73%)	-0.59	0 100 100	17, 40, 61, 69	0
All	All	731/988 (73%)	-0.61	2 (0%) 90 84	17, 41, 62, 80	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	VAL	3.0
1	C	132	GLU	2.8

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 oligosaccharides 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.