



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:21 PM UTC

PDB ID : 4WYV / pdb_00004wyv
Title : Crystal Structure of Human Translin in Open Conformation
Authors : Dvir, H.; Eliahoo, E.; Alian, A.
Deposited on : 2014-11-18
Resolution : 3.00 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

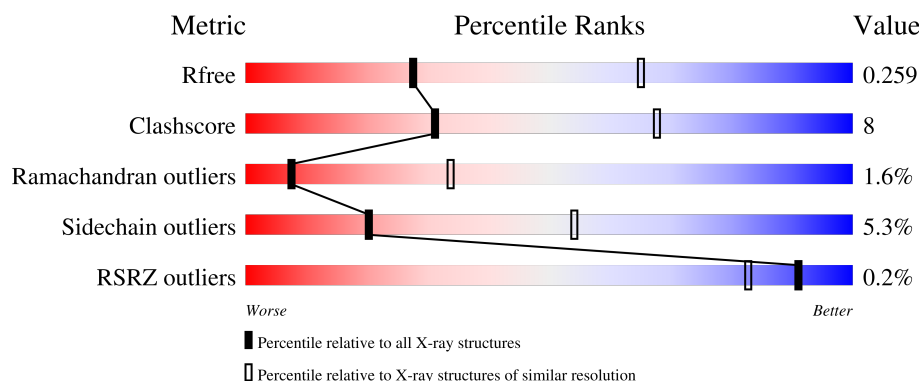
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	240	 70% 17% • 11%
1	B	240	 71% 16% • 12%
1	C	240	 68% 16% • 12%
1	D	240	 71% 15% • 11%
1	E	240	 67% 19% • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	240	 62%24%•12%
1	G	240	 67%20%•10%
1	H	240	 70%16%•12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13935 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 Translin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1741	1116	300	323	2			
1	B	212	Total	C	N	O	S	0	0	0
			1737	1114	299	322	2			
1	C	210	Total	C	N	O	S	0	0	0
			1717	1100	296	319	2			
1	D	214	Total	C	N	O	S	0	0	0
			1741	1113	301	325	2			
1	E	213	Total	C	N	O	S	0	0	0
			1743	1117	300	324	2			
1	F	212	Total	C	N	O	S	0	0	0
			1737	1114	299	322	2			
1	G	216	Total	C	N	O	S	0	0	0
			1767	1133	304	328	2			
1	H	212	Total	C	N	O	S	0	0	0
			1734	1112	298	322	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q15631
A	-10	ARG	-	expression tag	UNP Q15631
A	-9	GLY	-	expression tag	UNP Q15631
A	-8	SER	-	expression tag	UNP Q15631
A	-7	HIS	-	expression tag	UNP Q15631
A	-6	HIS	-	expression tag	UNP Q15631
A	-5	HIS	-	expression tag	UNP Q15631
A	-4	HIS	-	expression tag	UNP Q15631
A	-3	HIS	-	expression tag	UNP Q15631
A	-2	HIS	-	expression tag	UNP Q15631
A	-1	GLY	-	expression tag	UNP Q15631
A	0	SER	-	expression tag	UNP Q15631
B	-11	MET	-	initiating methionine	UNP Q15631

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	expression tag	UNP Q15631
B	-9	GLY	-	expression tag	UNP Q15631
B	-8	SER	-	expression tag	UNP Q15631
B	-7	HIS	-	expression tag	UNP Q15631
B	-6	HIS	-	expression tag	UNP Q15631
B	-5	HIS	-	expression tag	UNP Q15631
B	-4	HIS	-	expression tag	UNP Q15631
B	-3	HIS	-	expression tag	UNP Q15631
B	-2	HIS	-	expression tag	UNP Q15631
B	-1	GLY	-	expression tag	UNP Q15631
B	0	SER	-	expression tag	UNP Q15631
C	-11	MET	-	initiating methionine	UNP Q15631
C	-10	ARG	-	expression tag	UNP Q15631
C	-9	GLY	-	expression tag	UNP Q15631
C	-8	SER	-	expression tag	UNP Q15631
C	-7	HIS	-	expression tag	UNP Q15631
C	-6	HIS	-	expression tag	UNP Q15631
C	-5	HIS	-	expression tag	UNP Q15631
C	-4	HIS	-	expression tag	UNP Q15631
C	-3	HIS	-	expression tag	UNP Q15631
C	-2	HIS	-	expression tag	UNP Q15631
C	-1	GLY	-	expression tag	UNP Q15631
C	0	SER	-	expression tag	UNP Q15631
D	-11	MET	-	initiating methionine	UNP Q15631
D	-10	ARG	-	expression tag	UNP Q15631
D	-9	GLY	-	expression tag	UNP Q15631
D	-8	SER	-	expression tag	UNP Q15631
D	-7	HIS	-	expression tag	UNP Q15631
D	-6	HIS	-	expression tag	UNP Q15631
D	-5	HIS	-	expression tag	UNP Q15631
D	-4	HIS	-	expression tag	UNP Q15631
D	-3	HIS	-	expression tag	UNP Q15631
D	-2	HIS	-	expression tag	UNP Q15631
D	-1	GLY	-	expression tag	UNP Q15631
D	0	SER	-	expression tag	UNP Q15631
E	-11	MET	-	initiating methionine	UNP Q15631
E	-10	ARG	-	expression tag	UNP Q15631
E	-9	GLY	-	expression tag	UNP Q15631
E	-8	SER	-	expression tag	UNP Q15631
E	-7	HIS	-	expression tag	UNP Q15631
E	-6	HIS	-	expression tag	UNP Q15631
E	-5	HIS	-	expression tag	UNP Q15631

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q15631
E	-3	HIS	-	expression tag	UNP Q15631
E	-2	HIS	-	expression tag	UNP Q15631
E	-1	GLY	-	expression tag	UNP Q15631
E	0	SER	-	expression tag	UNP Q15631
F	-11	MET	-	initiating methionine	UNP Q15631
F	-10	ARG	-	expression tag	UNP Q15631
F	-9	GLY	-	expression tag	UNP Q15631
F	-8	SER	-	expression tag	UNP Q15631
F	-7	HIS	-	expression tag	UNP Q15631
F	-6	HIS	-	expression tag	UNP Q15631
F	-5	HIS	-	expression tag	UNP Q15631
F	-4	HIS	-	expression tag	UNP Q15631
F	-3	HIS	-	expression tag	UNP Q15631
F	-2	HIS	-	expression tag	UNP Q15631
F	-1	GLY	-	expression tag	UNP Q15631
F	0	SER	-	expression tag	UNP Q15631
G	-11	MET	-	initiating methionine	UNP Q15631
G	-10	ARG	-	expression tag	UNP Q15631
G	-9	GLY	-	expression tag	UNP Q15631
G	-8	SER	-	expression tag	UNP Q15631
G	-7	HIS	-	expression tag	UNP Q15631
G	-6	HIS	-	expression tag	UNP Q15631
G	-5	HIS	-	expression tag	UNP Q15631
G	-4	HIS	-	expression tag	UNP Q15631
G	-3	HIS	-	expression tag	UNP Q15631
G	-2	HIS	-	expression tag	UNP Q15631
G	-1	GLY	-	expression tag	UNP Q15631
G	0	SER	-	expression tag	UNP Q15631
H	-11	MET	-	initiating methionine	UNP Q15631
H	-10	ARG	-	expression tag	UNP Q15631
H	-9	GLY	-	expression tag	UNP Q15631
H	-8	SER	-	expression tag	UNP Q15631
H	-7	HIS	-	expression tag	UNP Q15631
H	-6	HIS	-	expression tag	UNP Q15631
H	-5	HIS	-	expression tag	UNP Q15631
H	-4	HIS	-	expression tag	UNP Q15631
H	-3	HIS	-	expression tag	UNP Q15631
H	-2	HIS	-	expression tag	UNP Q15631
H	-1	GLY	-	expression tag	UNP Q15631
H	0	SER	-	expression tag	UNP Q15631

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	2	Total 2	O 2	0	0
2	C	2	Total 2	O 2	0	0
2	D	2	Total 2	O 2	0	0
2	E	2	Total 2	O 2	0	0
2	F	2	Total 2	O 2	0	0
2	G	1	Total 1	O 1	0	0

- Molecule 1: Translin

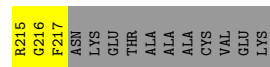




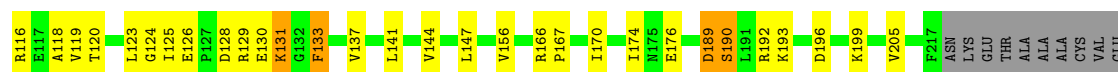
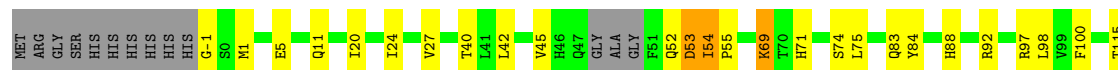
• Molecule 1: Translin



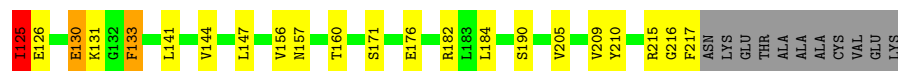
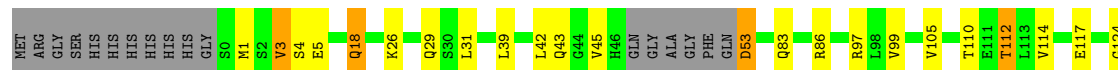
• Molecule 1: Translin



• Molecule 1: Translin



• Molecule 1: Translin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.31Å 82.31Å 635.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 3.00 58.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (58.00-3.00) 98.5 (58.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.272 0.215 , 0.259	Depositor DCC
R_{free} test set	2272 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13935	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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	0.99	1/1772 (0.1%)	1.00	3/2390 (0.1%)
1	B	0.98	1/1768 (0.1%)	1.04	2/2385 (0.1%)
1	C	1.05	3/1747 (0.2%)	0.99	1/2357 (0.0%)
1	D	0.94	0/1771	1.01	2/2389 (0.1%)
1	E	0.88	0/1774	0.95	0/2393
1	F	0.91	2/1768 (0.1%)	0.96	0/2385
1	G	1.04	4/1799 (0.2%)	1.00	2/2426 (0.1%)
1	H	0.93	1/1765 (0.1%)	0.99	2/2381 (0.1%)
All	All	0.97	12/14164 (0.1%)	0.99	12/19106 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	HIS	C-O	11.57	1.46	1.23
1	G	69	LYS	CG-CD	11.46	1.86	1.52
1	G	54	ILE	CA-CB	11.22	1.59	1.54
1	C	54	ILE	CA-CB	7.87	1.58	1.54
1	B	194	ARG	CZ-NH1	7.63	1.43	1.32
1	A	9	GLU	CD-OE1	7.18	1.39	1.25
1	H	4	SER	CB-OG	6.17	1.54	1.42
1	C	193	LYS	CG-CD	6.10	1.70	1.52
1	G	129	ARG	CZ-NH1	5.78	1.40	1.32
1	G	-1	GLY	N-CA	5.75	1.54	1.45
1	F	54	ILE	CA-CB	5.61	1.57	1.54
1	F	73	THR	CA-CB	5.41	1.62	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	124	GLY	N-CA-C	-7.08	102.85	111.35
1	C	133	PHE	N-CA-C	5.84	123.23	110.80
1	H	99	VAL	N-CA-C	-5.82	104.69	110.62
1	A	44	GLY	N-CA-C	-5.75	108.34	114.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	LYS	CA-C-N	5.59	128.33	120.28
1	D	76	LYS	C-N-CA	5.59	128.33	120.28
1	G	128	ASP	N-CA-C	5.51	118.05	111.71
1	G	54	ILE	N-CA-CB	5.38	114.13	110.52
1	B	59	LEU	CD1-CG-CD2	5.25	122.34	110.80
1	B	202	VAL	N-CA-C	-5.09	105.53	110.42
1	A	54	ILE	CA-C-N	-5.04	113.73	119.28
1	A	54	ILE	C-N-CA	-5.04	113.73	119.28

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	1741	0	1761	25	0
1	B	1737	0	1758	27	0
1	C	1717	0	1741	38	0
1	D	1741	0	1762	25	0
1	E	1743	0	1763	31	0
1	F	1737	0	1758	40	0
1	G	1767	0	1783	41	0
1	H	1734	0	1755	32	0
2	A	7	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
All	All	13935	0	14081	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (229) 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:G:69:LYS:CD	1:G:69:LYS:CG	1.86	1.50
1:F:110:THR:CG2	1:F:112:THR:HG22	1.81	1.09
1:F:110:THR:HG23	1:F:112:THR:HG22	1.37	1.03
1:E:72:LEU:HD23	1:E:125:ILE:HD11	1.52	0.91
1:C:39:LEU:HD11	1:C:43:GLN:HE21	1.43	0.83
1:B:80:PRO:HG2	1:B:83:GLN:HE21	1.44	0.82
1:B:183:LEU:HD11	1:F:8:VAL:HG22	1.62	0.82
1:E:1:MET:O	1:E:5:GLU:HB2	1.79	0.82
1:C:41:LEU:HB3	1:C:57:ARG:CZ	2.11	0.81
1:H:110:THR:OG1	1:H:112:THR:HG22	1.81	0.80
1:C:41:LEU:HB2	1:C:57:ARG:NH2	1.96	0.80
1:D:72:LEU:O	1:D:76:LYS:HG3	1.81	0.80
1:G:54:ILE:HG13	1:G:55:PRO:HD3	1.65	0.79
1:E:110:THR:OG1	1:E:112:THR:HG22	1.82	0.78
1:A:53:ASP:O	1:A:56:LYS:HB2	1.84	0.78
1:F:34:THR:O	1:F:38:ILE:HD12	1.86	0.76
1:D:74:SER:O	1:D:77:THR:HB	1.88	0.73
1:B:80:PRO:CG	1:B:83:GLN:HE21	2.00	0.73
1:C:110:THR:OG1	1:C:112:THR:HG22	1.89	0.72
1:B:210:TYR:O	1:B:214:ILE:HG22	1.90	0.72
1:G:69:LYS:CD	1:G:69:LYS:CB	2.67	0.72
1:F:110:THR:HG23	1:F:112:THR:CG2	2.15	0.72
1:F:110:THR:HG21	1:F:112:THR:HG22	1.73	0.71
1:C:41:LEU:CB	1:C:57:ARG:CZ	2.69	0.71
1:H:42:LEU:O	1:H:45:VAL:HG22	1.92	0.70
1:B:40:THR:HG23	1:C:182:ARG:HD2	1.74	0.70
1:A:36:ARG:HD2	1:B:182:ARG:O	1.93	0.68
1:D:110:THR:OG1	1:D:112:THR:HG22	1.92	0.68
1:F:215:ARG:HB2	1:F:217:PHE:HE1	1.58	0.68
1:F:34:THR:O	1:F:38:ILE:CD1	2.42	0.67
1:C:3:VAL:HG21	1:G:176:GLU:HB3	1.75	0.67
1:F:182:ARG:HD2	1:G:40:THR:HG23	1.78	0.66
1:B:42:LEU:O	1:B:45:VAL:HG13	1.96	0.65
1:H:39:LEU:HD21	1:H:43:GLN:CD	2.22	0.65
1:A:42:LEU:O	1:A:45:VAL:HG13	1.98	0.63
1:F:21:ARG:HH11	1:F:90:HIS:HE1	1.47	0.62
1:E:115:THR:HG23	1:E:118:ALA:H	1.65	0.62
1:B:117:GLU:O	1:B:120:THR:HG22	2.00	0.61
1:D:14:LEU:HD12	1:H:184:LEU:HD22	1.82	0.61
1:A:34:THR:O	1:A:38:ILE:HD12	2.01	0.61
1:E:72:LEU:CD2	1:E:125:ILE:HD11	2.30	0.60
1:F:53:ASP:O	1:F:56:LYS:HB2	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:SER:HA	1:D:168:LEU:HD12	1.81	0.60
1:A:53:ASP:HB2	1:A:56:LYS:HD3	1.84	0.60
1:A:115:THR:HG23	1:A:118:ALA:H	1.66	0.60
1:E:40:THR:HG23	1:H:182:ARG:HD2	1.84	0.59
1:C:3:VAL:CG2	1:G:176:GLU:HB3	2.32	0.59
1:C:41:LEU:HB3	1:C:57:ARG:NE	2.16	0.59
1:F:76:LYS:NZ	1:F:126:GLU:OE2	2.35	0.59
1:C:14:LEU:CD1	1:G:137:VAL:HG11	2.32	0.59
1:A:125:ILE:HG23	1:A:133:PHE:O	2.02	0.59
1:B:72:LEU:HD13	1:B:125:ILE:HD11	1.84	0.59
1:C:125:ILE:HG23	1:C:133:PHE:O	2.02	0.59
1:E:160:THR:HG21	1:H:209:VAL:HG12	1.84	0.59
1:C:41:LEU:CB	1:C:57:ARG:NH2	2.66	0.58
1:A:1:MET:HE2	1:A:5:GLU:HB3	1.84	0.58
1:H:1:MET:HE2	1:H:5:GLU:HB3	1.84	0.58
1:C:166:ARG:HB3	1:C:167:PRO:HD3	1.85	0.58
1:C:156:VAL:O	1:C:159:VAL:HG12	2.04	0.58
1:F:156:VAL:HG21	1:F:204:LYS:HE2	1.85	0.58
1:G:125:ILE:HG22	1:G:126:GLU:N	2.18	0.58
1:H:110:THR:HG1	1:H:112:THR:HG22	1.67	0.57
1:B:171:SER:HA	1:B:205:VAL:HG11	1.88	0.56
1:F:21:ARG:HH11	1:F:90:HIS:CE1	2.23	0.56
1:F:128:ASP:HA	1:F:134:HIS:CD2	2.39	0.56
1:G:125:ILE:HG23	1:G:133:PHE:O	2.05	0.56
1:B:215:ARG:CZ	1:C:214:ILE:HD12	2.36	0.56
1:C:125:ILE:HG22	1:C:126:GLU:N	2.20	0.56
1:B:165:SER:HA	1:B:168:LEU:HD12	1.88	0.56
1:B:184:LEU:HD22	1:F:14:LEU:HD12	1.87	0.55
1:B:210:TYR:O	1:B:214:ILE:CG2	2.53	0.55
1:H:39:LEU:C	1:H:39:LEU:HD23	2.32	0.55
1:G:52:GLN:O	1:G:53:ASP:HB3	2.06	0.54
1:C:41:LEU:C	1:C:57:ARG:HE	2.15	0.54
1:C:147:LEU:HD22	1:C:151:LEU:HG	1.89	0.54
1:D:116:ARG:O	1:D:120:THR:HG23	2.08	0.54
1:E:45:VAL:HG23	1:E:54:ILE:HD11	1.90	0.54
1:G:166:ARG:HB3	1:G:167:PRO:HD3	1.90	0.53
1:E:174:ILE:HG22	1:E:202:VAL:HG22	1.90	0.53
1:F:24:ILE:O	1:F:28:VAL:HG23	2.08	0.53
1:F:184:LEU:HD23	1:F:186:LEU:HD21	1.90	0.53
1:A:125:ILE:HG22	1:A:126:GLU:N	2.24	0.53
1:H:125:ILE:HD13	1:H:125:ILE:N	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ILE:HG22	1:E:126:GLU:N	2.24	0.52
1:G:42:LEU:O	1:G:45:VAL:HG13	2.08	0.52
1:G:69:LYS:CG	1:G:69:LYS:CE	2.80	0.52
1:H:53:ASP:OD1	1:H:53:ASP:C	2.52	0.52
1:H:171:SER:HA	1:H:205:VAL:HG11	1.92	0.52
1:D:125:ILE:HG22	1:D:126:GLU:N	2.23	0.52
1:A:28:VAL:O	1:A:32:GLU:HG3	2.10	0.52
1:G:1:MET:HE2	1:G:5:GLU:HB3	1.93	0.52
1:A:125:ILE:CG2	1:A:133:PHE:O	2.59	0.51
1:H:125:ILE:HG22	1:H:126:GLU:N	2.25	0.51
1:E:180:GLY:O	1:E:183:LEU:HB2	2.10	0.51
1:G:52:GLN:O	1:G:52:GLN:HG2	2.10	0.51
1:A:53:ASP:OD1	1:A:53:ASP:C	2.54	0.51
1:G:190:SER:O	1:G:193:LYS:HE2	2.11	0.51
1:D:3:VAL:HG21	1:H:176:GLU:HB3	1.93	0.50
1:A:171:SER:HA	1:A:205:VAL:HG11	1.93	0.50
1:D:77:THR:HG22	1:D:78:LYS:HD3	1.94	0.50
1:F:9:GLU:HG2	1:F:13:PHE:HE2	1.77	0.50
1:D:174:ILE:HG22	1:D:202:VAL:HG22	1.94	0.50
1:E:160:THR:CG2	1:H:209:VAL:HG12	2.42	0.50
1:F:141:LEU:HD12	1:F:191:LEU:HD21	1.94	0.50
1:D:196:ASP:O	1:D:199:LYS:HG2	2.12	0.50
1:F:131:LYS:HD2	1:F:134:HIS:HE1	1.76	0.50
1:A:189:ASP:OD1	1:A:192:ARG:NH2	2.46	0.49
1:B:1:MET:HE2	1:B:5:GLU:HB3	1.95	0.49
1:E:129:ARG:HH11	1:E:129:ARG:HB3	1.77	0.49
1:E:115:THR:CG2	1:E:118:ALA:HB2	2.42	0.48
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.78	0.48
1:A:27:VAL:HG13	1:A:75:LEU:HD13	1.95	0.48
1:H:125:ILE:HG23	1:H:133:PHE:O	2.13	0.48
1:C:184:LEU:HA	1:G:11:GLN:OE1	2.14	0.48
1:F:215:ARG:HB2	1:F:217:PHE:CE1	2.43	0.48
1:A:184:LEU:HD22	1:E:14:LEU:HD12	1.95	0.48
1:D:4:SER:O	1:D:8:VAL:HG13	2.14	0.48
1:H:157:ASN:O	1:H:160:THR:HB	2.13	0.48
1:G:71:HIS:O	1:G:74:SER:HB3	2.14	0.48
1:E:66:GLY:HA2	1:E:69:LYS:NZ	2.29	0.47
1:C:14:LEU:HD11	1:G:137:VAL:HG11	1.96	0.47
1:D:187:LYS:HG3	1:H:18:GLN:HG2	1.95	0.47
1:F:116:ARG:O	1:F:120:THR:HG23	2.14	0.47
1:D:10:LEU:HD13	1:H:141:LEU:HD21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ILE:CG2	1:G:126:GLU:N	2.77	0.47
1:F:38:ILE:HD11	1:F:64:HIS:HB3	1.95	0.47
1:D:125:ILE:CG2	1:D:126:GLU:N	2.77	0.47
1:E:39:LEU:HD11	1:E:43:GLN:HE21	1.80	0.47
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.74	0.47
1:C:5:GLU:O	1:C:8:VAL:HG12	2.13	0.47
1:C:115:THR:HG23	1:C:118:ALA:H	1.80	0.46
1:C:72:LEU:HD13	1:C:125:ILE:HD11	1.96	0.46
1:C:30:SER:O	1:C:34:THR:HG22	2.14	0.46
1:A:163:ASP:C	1:A:163:ASP:OD1	2.59	0.46
1:C:125:ILE:CG2	1:C:126:GLU:N	2.78	0.46
1:G:69:LYS:HG3	1:G:124:GLY:HA3	1.98	0.46
1:B:36:ARG:HD2	1:C:182:ARG:O	2.16	0.46
1:G:115:THR:HG23	1:G:118:ALA:H	1.81	0.45
1:H:117:GLU:CD	1:H:117:GLU:H	2.23	0.45
1:G:88:HIS:HE1	1:G:92:ARG:NH1	2.14	0.45
1:H:125:ILE:HD13	1:H:125:ILE:H	1.82	0.45
1:H:114:VAL:HG13	1:H:114:VAL:O	2.17	0.45
1:G:98:LEU:HB3	1:G:123:LEU:HD21	1.98	0.45
1:H:42:LEU:HD11	1:H:105:VAL:HG23	1.98	0.45
1:F:38:ILE:HD12	1:F:38:ILE:H	1.80	0.45
1:C:10:LEU:HD13	1:G:141:LEU:HD21	1.99	0.45
1:H:83:GLN:OE1	1:H:86:ARG:HD2	2.17	0.45
1:A:130:GLU:O	1:A:131:LYS:O	2.35	0.44
1:F:91:TRP:O	1:F:95:LEU:HB2	2.17	0.44
1:G:69:LYS:CD	1:G:69:LYS:HB3	2.43	0.44
1:C:14:LEU:HD11	1:G:137:VAL:CG1	2.48	0.44
1:H:126:GLU:HB3	1:H:130:GLU:HB3	2.00	0.44
1:F:88:HIS:HA	1:F:91:TRP:CZ2	2.52	0.44
1:F:106:VAL:O	1:F:110:THR:HG22	2.17	0.44
1:B:80:PRO:HG3	1:B:83:GLN:HE21	1.82	0.44
1:E:66:GLY:HA2	1:E:69:LYS:HZ2	1.83	0.44
1:E:115:THR:HG23	1:E:118:ALA:CB	2.47	0.44
1:E:126:GLU:HB3	1:E:130:GLU:HB3	1.98	0.44
1:E:196:ASP:O	1:E:199:LYS:HG2	2.17	0.44
1:F:2:SER:O	1:F:6:ILE:HG13	2.17	0.44
1:F:212:LEU:O	1:F:217:PHE:HD1	2.01	0.44
1:A:166:ARG:HB3	1:A:167:PRO:HD3	2.00	0.43
1:D:176:GLU:HB3	1:H:3:VAL:HG21	1.99	0.43
1:E:132:GLY:O	1:E:133:PHE:C	2.61	0.43
1:H:215:ARG:C	1:H:217:PHE:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:THR:CG2	1:C:182:ARG:HD2	2.45	0.43
1:B:103:ALA:HB1	1:B:147:LEU:HD22	2.00	0.43
1:E:41:LEU:HD21	1:E:60:LYS:HB3	2.00	0.43
1:D:42:LEU:HD11	1:D:105:VAL:HG23	2.01	0.43
1:G:100:PHE:CD1	1:G:100:PHE:C	2.97	0.43
1:G:116:ARG:O	1:G:120:THR:HG23	2.18	0.43
1:H:144:VAL:O	1:H:147:LEU:HB3	2.18	0.43
1:G:126:GLU:HB3	1:G:130:GLU:HB3	2.01	0.43
1:H:26:LYS:O	1:H:29:GLN:HB2	2.19	0.43
1:A:211:ASP:HB3	1:B:214:ILE:HD12	2.01	0.43
1:F:131:LYS:HD2	1:F:131:LYS:HA	1.85	0.43
1:G:196:ASP:O	1:G:199:LYS:HG2	2.19	0.43
1:F:84:TYR:HD1	1:F:85:TYR:CD1	2.37	0.43
1:C:171:SER:HA	1:C:205:VAL:HG11	2.01	0.42
1:E:72:LEU:HD23	1:E:125:ILE:CD1	2.36	0.42
1:C:41:LEU:HB2	1:C:57:ARG:CZ	2.41	0.42
1:G:20:ILE:O	1:G:24:ILE:HG13	2.19	0.42
1:B:54:ILE:N	1:B:55:PRO:CD	2.83	0.42
1:E:117:GLU:O	1:E:120:THR:HB	2.19	0.42
1:A:20:ILE:O	1:A:24:ILE:HG13	2.20	0.42
1:D:166:ARG:HB3	1:D:167:PRO:HD3	2.00	0.42
1:C:119:VAL:O	1:C:123:LEU:HG	2.20	0.42
1:C:163:ASP:C	1:C:163:ASP:OD1	2.63	0.42
1:D:210:TYR:CZ	1:D:214:ILE:HD12	2.54	0.42
1:G:144:VAL:O	1:G:147:LEU:HB3	2.19	0.42
1:A:5:GLU:O	1:A:8:VAL:HG22	2.19	0.42
1:F:74:SER:O	1:F:77:THR:HB	2.19	0.42
1:G:125:ILE:CG2	1:G:133:PHE:O	2.68	0.42
1:F:110:THR:CG2	1:F:112:THR:CG2	2.73	0.42
1:A:14:LEU:HD11	1:E:137:VAL:HG21	2.02	0.42
1:A:14:LEU:HD22	1:E:184:LEU:HD22	2.02	0.42
1:D:117:GLU:O	1:D:120:THR:OG1	2.27	0.42
1:G:170:ILE:HG22	1:G:205:VAL:HG21	2.02	0.42
1:H:171:SER:HA	1:H:205:VAL:CG1	2.50	0.42
1:C:14:LEU:HD13	1:G:137:VAL:HG11	2.00	0.41
1:G:88:HIS:CE1	1:G:92:ARG:NH1	2.88	0.41
1:D:117:GLU:H	1:D:117:GLU:CD	2.29	0.41
1:B:83:GLN:O	1:B:86:ARG:HB2	2.21	0.41
1:F:25:ARG:HE	1:F:90:HIS:CD2	2.37	0.41
1:B:42:LEU:HD11	1:B:105:VAL:HG23	2.01	0.41
1:E:59:LEU:HD23	1:E:59:LEU:HA	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ASP:HA	1:F:134:HIS:HD2	1.81	0.41
1:C:39:LEU:CD1	1:C:43:GLN:HE21	2.24	0.41
1:D:179:SER:O	1:D:182:ARG:HB2	2.21	0.41
1:F:210:TYR:CD2	1:G:156:VAL:HG13	2.56	0.41
1:B:125:ILE:HG23	1:B:133:PHE:O	2.21	0.41
1:C:76:LYS:NZ	1:C:126:GLU:OE2	2.53	0.41
1:E:88:HIS:HA	1:E:91:TRP:CZ2	2.55	0.41
1:F:166:ARG:HB3	1:F:167:PRO:HD3	2.03	0.41
1:G:27:VAL:HG11	1:G:75:LEU:HB2	2.03	0.41
1:G:83:GLN:O	1:G:84:TYR:C	2.64	0.41
1:A:102:ALA:O	1:A:105:VAL:HG22	2.20	0.41
1:D:125:ILE:HG23	1:D:133:PHE:O	2.20	0.41
1:F:41:LEU:O	1:F:57:ARG:NH1	2.54	0.41
1:F:34:THR:O	1:F:38:ILE:HD13	2.21	0.40
1:B:160:THR:CG2	1:C:209:VAL:HG12	2.52	0.40
1:D:98:LEU:HB3	1:D:123:LEU:HD21	2.03	0.40
1:E:103:ALA:HB1	1:E:147:LEU:HD22	2.03	0.40
1:G:189:ASP:OD1	1:G:192:ARG:NH2	2.54	0.40
1:H:39:LEU:HD21	1:H:43:GLN:OE1	2.22	0.40
1:H:210:TYR:CD1	1:H:210:TYR:C	3.00	0.40
1:C:22:GLU:OE1	1:C:22:GLU:HA	2.21	0.40
1:D:47:GLN:O	1:D:49:ALA:N	2.55	0.40
1:E:4:SER:O	1:E:8:VAL:HG23	2.21	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	209/240 (87%)	201 (96%)	4 (2%)	4 (2%)	6	30
1	B	208/240 (87%)	202 (97%)	4 (2%)	2 (1%)	12	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	206/240 (86%)	198 (96%)	6 (3%)	2 (1%)	12	45
1	D	210/240 (88%)	202 (96%)	4 (2%)	4 (2%)	6	30
1	E	209/240 (87%)	199 (95%)	5 (2%)	5 (2%)	4	24
1	F	208/240 (87%)	201 (97%)	4 (2%)	3 (1%)	9	36
1	G	212/240 (88%)	204 (96%)	5 (2%)	3 (1%)	9	36
1	H	208/240 (87%)	199 (96%)	5 (2%)	4 (2%)	6	30
All	All	1670/1920 (87%)	1606 (96%)	37 (2%)	27 (2%)	7	34

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	133	PHE
1	B	133	PHE
1	C	133	PHE
1	D	133	PHE
1	F	131	LYS
1	F	133	PHE
1	G	53	ASP
1	G	133	PHE
1	H	125	ILE
1	H	131	LYS
1	H	133	PHE
1	C	131	LYS
1	D	48	GLY
1	D	136	ASP
1	E	2	SER
1	E	133	PHE
1	G	131	LYS
1	A	136	ASP
1	A	216	GLY
1	D	131	LYS
1	E	131	LYS
1	E	136	ASP
1	F	216	GLY
1	B	216	GLY
1	E	216	GLY
1	H	216	GLY

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	192/212 (91%)	183 (95%)	9 (5%)	23	58
1	B	192/212 (91%)	182 (95%)	10 (5%)	21	55
1	C	190/212 (90%)	178 (94%)	12 (6%)	16	48
1	D	192/212 (91%)	183 (95%)	9 (5%)	23	58
1	E	193/212 (91%)	180 (93%)	13 (7%)	15	46
1	F	192/212 (91%)	179 (93%)	13 (7%)	14	45
1	G	195/212 (92%)	189 (97%)	6 (3%)	35	68
1	H	192/212 (91%)	182 (95%)	10 (5%)	21	55
All	All	1538/1696 (91%)	1456 (95%)	82 (5%)	20	54

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	VAL
1	A	14	LEU
1	A	31	LEU
1	A	38	ILE
1	A	53	ASP
1	A	168	LEU
1	A	174	ILE
1	A	190	SER
1	B	3	VAL
1	B	29	GLN
1	B	86	ARG
1	B	97	ARG
1	B	115	THR
1	B	131	LYS
1	B	174	ILE
1	B	190	SER
1	B	194	ARG
1	B	214	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3	VAL
1	C	14	LEU
1	C	18	GLN
1	C	31	LEU
1	C	34	THR
1	C	53	ASP
1	C	97	ARG
1	C	112	THR
1	C	147	LEU
1	C	159	VAL
1	C	168	LEU
1	C	190	SER
1	D	3	VAL
1	D	8	VAL
1	D	33	GLN
1	D	47	GLN
1	D	97	ARG
1	D	112	THR
1	D	174	ILE
1	D	190	SER
1	D	214	ILE
1	E	3	VAL
1	E	31	LEU
1	E	40	THR
1	E	95	LEU
1	E	97	ARG
1	E	112	THR
1	E	129	ARG
1	E	131	LYS
1	E	137	VAL
1	E	151	LEU
1	E	174	ILE
1	E	190	SER
1	E	205	VAL
1	F	3	VAL
1	F	27	VAL
1	F	31	LEU
1	F	40	THR
1	F	41	LEU
1	F	63	GLU
1	F	67	THR
1	F	68	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	95	LEU
1	F	97	ARG
1	F	112	THR
1	F	174	ILE
1	F	190	SER
1	G	97	ARG
1	G	119	VAL
1	G	131	LYS
1	G	174	ILE
1	G	189	ASP
1	G	190	SER
1	H	3	VAL
1	H	18	GLN
1	H	31	LEU
1	H	53	ASP
1	H	97	ARG
1	H	112	THR
1	H	125	ILE
1	H	130	GLU
1	H	156	VAL
1	H	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	GLN
1	B	83	GLN
1	B	169	HIS
1	B	175	ASN
1	C	18	GLN
1	C	43	GLN
1	C	175	ASN
1	D	11	GLN
1	D	47	GLN
1	E	29	GLN
1	E	83	GLN
1	E	175	ASN
1	F	11	GLN
1	F	47	GLN
1	F	90	HIS
1	F	134	HIS
1	F	175	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	18	GLN
1	H	11	GLN
1	H	46	HIS
1	H	83	GLN
1	H	157	ASN
1	H	175	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	213/240 (88%)	-0.56	1 (0%) 87 72	40, 72, 106, 127	0
1	B	212/240 (88%)	-0.59	0 100 100	44, 74, 104, 128	0
1	C	210/240 (87%)	-0.50	1 (0%) 87 72	46, 80, 112, 125	0
1	D	214/240 (89%)	-0.52	2 (0%) 81 61	47, 73, 109, 131	0
1	E	213/240 (88%)	-0.46	0 100 100	59, 85, 114, 134	0
1	F	212/240 (88%)	-0.45	0 100 100	60, 91, 122, 136	0
1	G	216/240 (90%)	-0.54	0 100 100	50, 79, 110, 132	0
1	H	212/240 (88%)	-0.39	0 100 100	59, 85, 105, 121	0
All	All	1702/1920 (88%)	-0.50	4 (0%) 91 83	40, 81, 112, 136	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	ALA	2.5
1	D	216	GLY	2.1
1	A	48	GLY	2.1
1	C	216	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.