



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:06 AM UTC

PDB ID : 4DG7 / pdb_00004dg7
Title : Low resolution structure of Drosophila Translin
Authors : Kumar, V.; Gupta, G.D.
Deposited on : 2012-01-25
Resolution : 4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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:

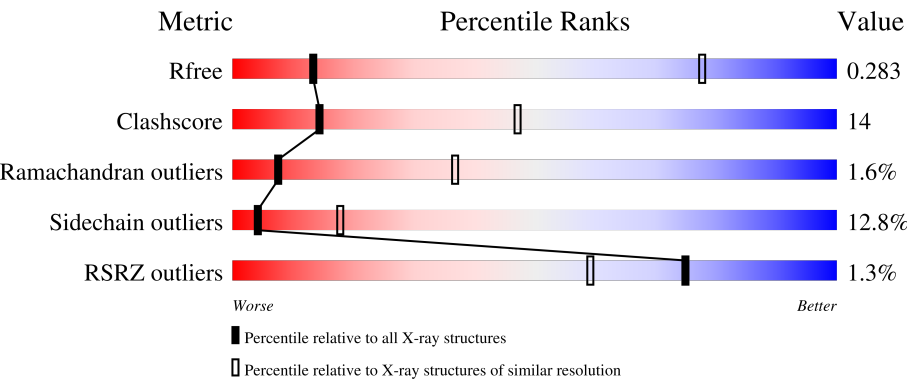
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	255	2% 49% 28% 5% 17%
1	B	255	2% 50% 29% • 16%
1	C	255	2% 51% 28% • 17%
1	D	255	% 54% 25% • 16%
1	E	255	% 51% 28% • 15%

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Mol	Chain	Length	Quality of chain
1	F	255	51%29%•16%
1	G	255	% 52%25%6%•16%
1	H	255	% 50%29%5%•15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13931 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	212	Total	C	N	O	S	0	0	0
			1727	1108	294	321	4			
1	B	213	Total	C	N	O	S	0	0	0
			1731	1108	295	324	4			
1	C	212	Total	C	N	O	S	0	0	0
			1727	1108	294	321	4			
1	D	214	Total	C	N	O	S	0	0	0
			1739	1114	296	325	4			
1	E	216	Total	C	N	O	S	0	0	0
			1757	1125	299	329	4			
1	F	215	Total	C	N	O	S	0	0	0
			1748	1120	298	326	4			
1	G	214	Total	C	N	O	S	0	0	0
			1739	1114	296	325	4			
1	H	217	Total	C	N	O	S	0	0	0
			1763	1129	301	329	4			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q7JVK6
A	-18	GLY	-	expression tag	UNP Q7JVK6
A	-17	SER	-	expression tag	UNP Q7JVK6
A	-16	SER	-	expression tag	UNP Q7JVK6
A	-15	HIS	-	expression tag	UNP Q7JVK6
A	-14	HIS	-	expression tag	UNP Q7JVK6
A	-13	HIS	-	expression tag	UNP Q7JVK6
A	-12	HIS	-	expression tag	UNP Q7JVK6
A	-11	HIS	-	expression tag	UNP Q7JVK6
A	-10	HIS	-	expression tag	UNP Q7JVK6
A	-9	SER	-	expression tag	UNP Q7JVK6
A	-8	SER	-	expression tag	UNP Q7JVK6
A	-7	GLY	-	expression tag	UNP Q7JVK6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q7JVK6
A	-5	VAL	-	expression tag	UNP Q7JVK6
A	-4	PRO	-	expression tag	UNP Q7JVK6
A	-3	ARG	-	expression tag	UNP Q7JVK6
A	-2	GLY	-	expression tag	UNP Q7JVK6
A	-1	SER	-	expression tag	UNP Q7JVK6
A	0	HIS	-	expression tag	UNP Q7JVK6
B	-19	MET	-	expression tag	UNP Q7JVK6
B	-18	GLY	-	expression tag	UNP Q7JVK6
B	-17	SER	-	expression tag	UNP Q7JVK6
B	-16	SER	-	expression tag	UNP Q7JVK6
B	-15	HIS	-	expression tag	UNP Q7JVK6
B	-14	HIS	-	expression tag	UNP Q7JVK6
B	-13	HIS	-	expression tag	UNP Q7JVK6
B	-12	HIS	-	expression tag	UNP Q7JVK6
B	-11	HIS	-	expression tag	UNP Q7JVK6
B	-10	HIS	-	expression tag	UNP Q7JVK6
B	-9	SER	-	expression tag	UNP Q7JVK6
B	-8	SER	-	expression tag	UNP Q7JVK6
B	-7	GLY	-	expression tag	UNP Q7JVK6
B	-6	LEU	-	expression tag	UNP Q7JVK6
B	-5	VAL	-	expression tag	UNP Q7JVK6
B	-4	PRO	-	expression tag	UNP Q7JVK6
B	-3	ARG	-	expression tag	UNP Q7JVK6
B	-2	GLY	-	expression tag	UNP Q7JVK6
B	-1	SER	-	expression tag	UNP Q7JVK6
B	0	HIS	-	expression tag	UNP Q7JVK6
C	-19	MET	-	expression tag	UNP Q7JVK6
C	-18	GLY	-	expression tag	UNP Q7JVK6
C	-17	SER	-	expression tag	UNP Q7JVK6
C	-16	SER	-	expression tag	UNP Q7JVK6
C	-15	HIS	-	expression tag	UNP Q7JVK6
C	-14	HIS	-	expression tag	UNP Q7JVK6
C	-13	HIS	-	expression tag	UNP Q7JVK6
C	-12	HIS	-	expression tag	UNP Q7JVK6
C	-11	HIS	-	expression tag	UNP Q7JVK6
C	-10	HIS	-	expression tag	UNP Q7JVK6
C	-9	SER	-	expression tag	UNP Q7JVK6
C	-8	SER	-	expression tag	UNP Q7JVK6
C	-7	GLY	-	expression tag	UNP Q7JVK6
C	-6	LEU	-	expression tag	UNP Q7JVK6
C	-5	VAL	-	expression tag	UNP Q7JVK6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q7JVK6
C	-3	ARG	-	expression tag	UNP Q7JVK6
C	-2	GLY	-	expression tag	UNP Q7JVK6
C	-1	SER	-	expression tag	UNP Q7JVK6
C	0	HIS	-	expression tag	UNP Q7JVK6
D	-19	MET	-	expression tag	UNP Q7JVK6
D	-18	GLY	-	expression tag	UNP Q7JVK6
D	-17	SER	-	expression tag	UNP Q7JVK6
D	-16	SER	-	expression tag	UNP Q7JVK6
D	-15	HIS	-	expression tag	UNP Q7JVK6
D	-14	HIS	-	expression tag	UNP Q7JVK6
D	-13	HIS	-	expression tag	UNP Q7JVK6
D	-12	HIS	-	expression tag	UNP Q7JVK6
D	-11	HIS	-	expression tag	UNP Q7JVK6
D	-10	HIS	-	expression tag	UNP Q7JVK6
D	-9	SER	-	expression tag	UNP Q7JVK6
D	-8	SER	-	expression tag	UNP Q7JVK6
D	-7	GLY	-	expression tag	UNP Q7JVK6
D	-6	LEU	-	expression tag	UNP Q7JVK6
D	-5	VAL	-	expression tag	UNP Q7JVK6
D	-4	PRO	-	expression tag	UNP Q7JVK6
D	-3	ARG	-	expression tag	UNP Q7JVK6
D	-2	GLY	-	expression tag	UNP Q7JVK6
D	-1	SER	-	expression tag	UNP Q7JVK6
D	0	HIS	-	expression tag	UNP Q7JVK6
E	-19	MET	-	expression tag	UNP Q7JVK6
E	-18	GLY	-	expression tag	UNP Q7JVK6
E	-17	SER	-	expression tag	UNP Q7JVK6
E	-16	SER	-	expression tag	UNP Q7JVK6
E	-15	HIS	-	expression tag	UNP Q7JVK6
E	-14	HIS	-	expression tag	UNP Q7JVK6
E	-13	HIS	-	expression tag	UNP Q7JVK6
E	-12	HIS	-	expression tag	UNP Q7JVK6
E	-11	HIS	-	expression tag	UNP Q7JVK6
E	-10	HIS	-	expression tag	UNP Q7JVK6
E	-9	SER	-	expression tag	UNP Q7JVK6
E	-8	SER	-	expression tag	UNP Q7JVK6
E	-7	GLY	-	expression tag	UNP Q7JVK6
E	-6	LEU	-	expression tag	UNP Q7JVK6
E	-5	VAL	-	expression tag	UNP Q7JVK6
E	-4	PRO	-	expression tag	UNP Q7JVK6
E	-3	ARG	-	expression tag	UNP Q7JVK6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q7JVK6
E	-1	SER	-	expression tag	UNP Q7JVK6
E	0	HIS	-	expression tag	UNP Q7JVK6
F	-19	MET	-	expression tag	UNP Q7JVK6
F	-18	GLY	-	expression tag	UNP Q7JVK6
F	-17	SER	-	expression tag	UNP Q7JVK6
F	-16	SER	-	expression tag	UNP Q7JVK6
F	-15	HIS	-	expression tag	UNP Q7JVK6
F	-14	HIS	-	expression tag	UNP Q7JVK6
F	-13	HIS	-	expression tag	UNP Q7JVK6
F	-12	HIS	-	expression tag	UNP Q7JVK6
F	-11	HIS	-	expression tag	UNP Q7JVK6
F	-10	HIS	-	expression tag	UNP Q7JVK6
F	-9	SER	-	expression tag	UNP Q7JVK6
F	-8	SER	-	expression tag	UNP Q7JVK6
F	-7	GLY	-	expression tag	UNP Q7JVK6
F	-6	LEU	-	expression tag	UNP Q7JVK6
F	-5	VAL	-	expression tag	UNP Q7JVK6
F	-4	PRO	-	expression tag	UNP Q7JVK6
F	-3	ARG	-	expression tag	UNP Q7JVK6
F	-2	GLY	-	expression tag	UNP Q7JVK6
F	-1	SER	-	expression tag	UNP Q7JVK6
F	0	HIS	-	expression tag	UNP Q7JVK6
G	-19	MET	-	expression tag	UNP Q7JVK6
G	-18	GLY	-	expression tag	UNP Q7JVK6
G	-17	SER	-	expression tag	UNP Q7JVK6
G	-16	SER	-	expression tag	UNP Q7JVK6
G	-15	HIS	-	expression tag	UNP Q7JVK6
G	-14	HIS	-	expression tag	UNP Q7JVK6
G	-13	HIS	-	expression tag	UNP Q7JVK6
G	-12	HIS	-	expression tag	UNP Q7JVK6
G	-11	HIS	-	expression tag	UNP Q7JVK6
G	-10	HIS	-	expression tag	UNP Q7JVK6
G	-9	SER	-	expression tag	UNP Q7JVK6
G	-8	SER	-	expression tag	UNP Q7JVK6
G	-7	GLY	-	expression tag	UNP Q7JVK6
G	-6	LEU	-	expression tag	UNP Q7JVK6
G	-5	VAL	-	expression tag	UNP Q7JVK6
G	-4	PRO	-	expression tag	UNP Q7JVK6
G	-3	ARG	-	expression tag	UNP Q7JVK6
G	-2	GLY	-	expression tag	UNP Q7JVK6
G	-1	SER	-	expression tag	UNP Q7JVK6

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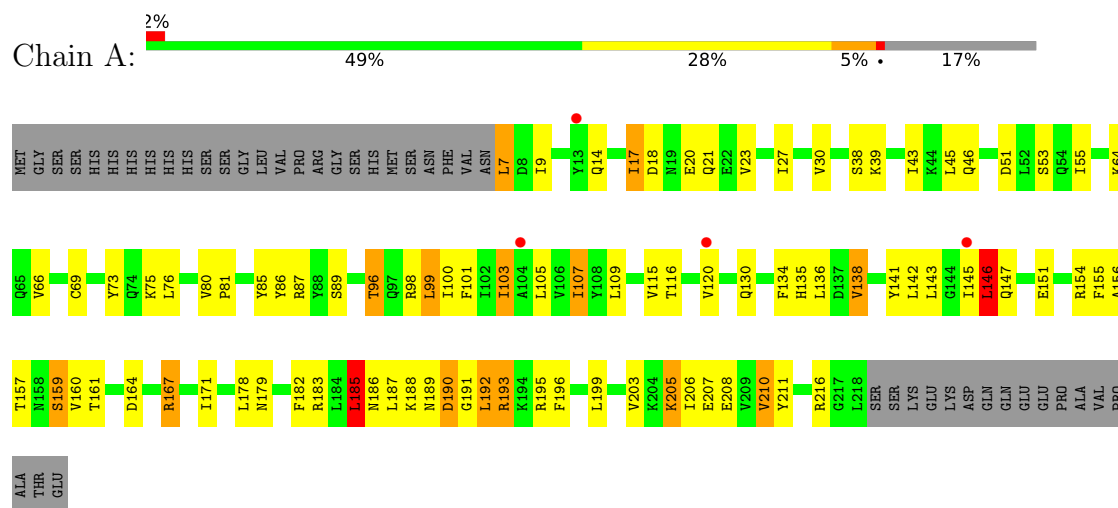
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q7JVK6
H	-19	MET	-	expression tag	UNP Q7JVK6
H	-18	GLY	-	expression tag	UNP Q7JVK6
H	-17	SER	-	expression tag	UNP Q7JVK6
H	-16	SER	-	expression tag	UNP Q7JVK6
H	-15	HIS	-	expression tag	UNP Q7JVK6
H	-14	HIS	-	expression tag	UNP Q7JVK6
H	-13	HIS	-	expression tag	UNP Q7JVK6
H	-12	HIS	-	expression tag	UNP Q7JVK6
H	-11	HIS	-	expression tag	UNP Q7JVK6
H	-10	HIS	-	expression tag	UNP Q7JVK6
H	-9	SER	-	expression tag	UNP Q7JVK6
H	-8	SER	-	expression tag	UNP Q7JVK6
H	-7	GLY	-	expression tag	UNP Q7JVK6
H	-6	LEU	-	expression tag	UNP Q7JVK6
H	-5	VAL	-	expression tag	UNP Q7JVK6
H	-4	PRO	-	expression tag	UNP Q7JVK6
H	-3	ARG	-	expression tag	UNP Q7JVK6
H	-2	GLY	-	expression tag	UNP Q7JVK6
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H	0	HIS	-	expression tag	UNP Q7JVK6

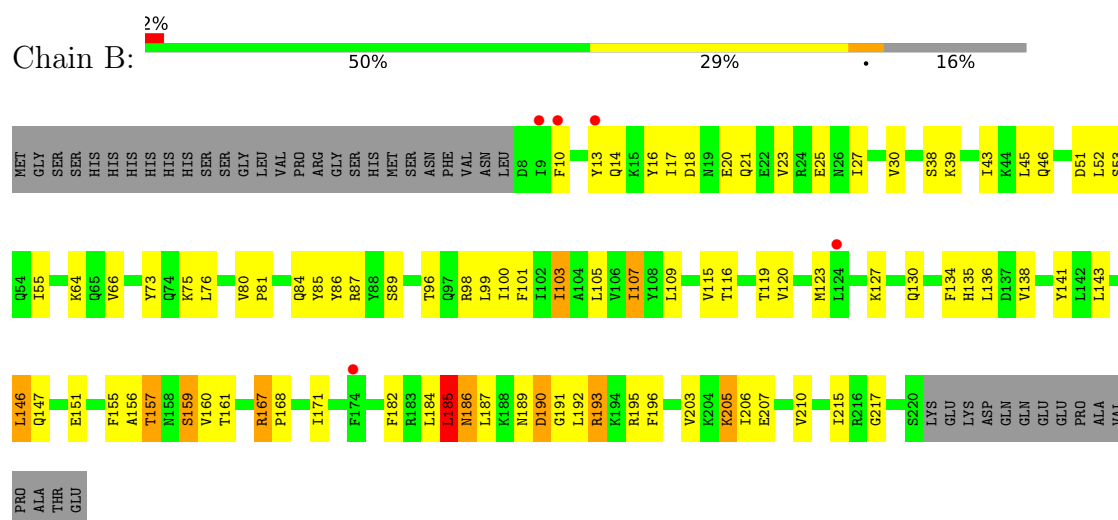
3 Residue-property plots [i](#)

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

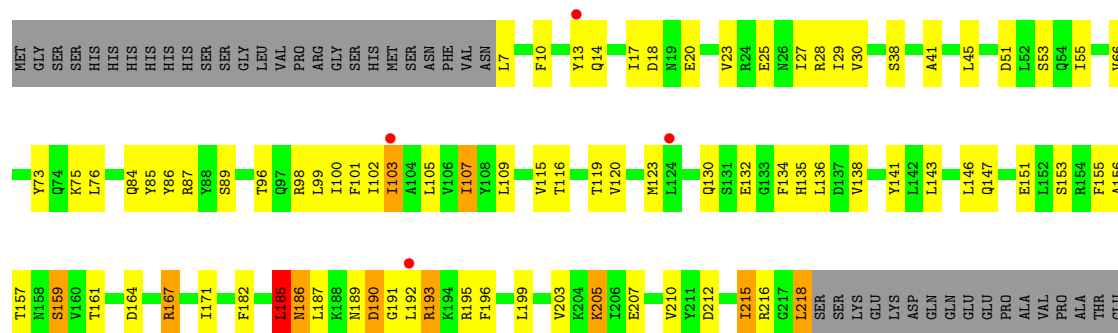


• Molecule 1: GM27569p

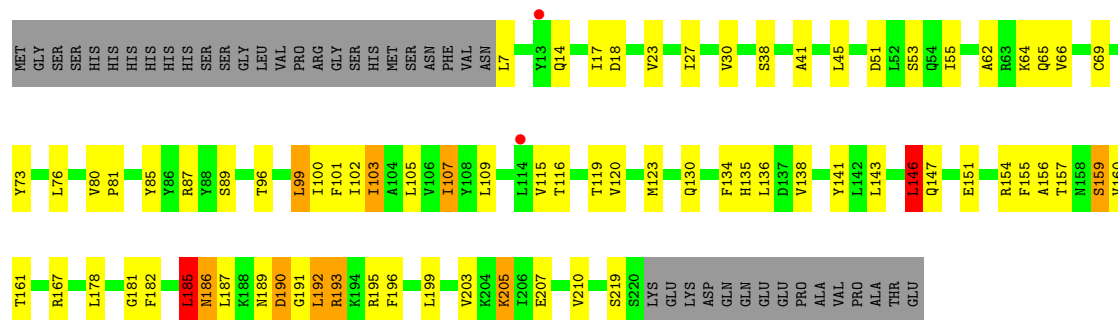


• Molecule 1: GM27569p

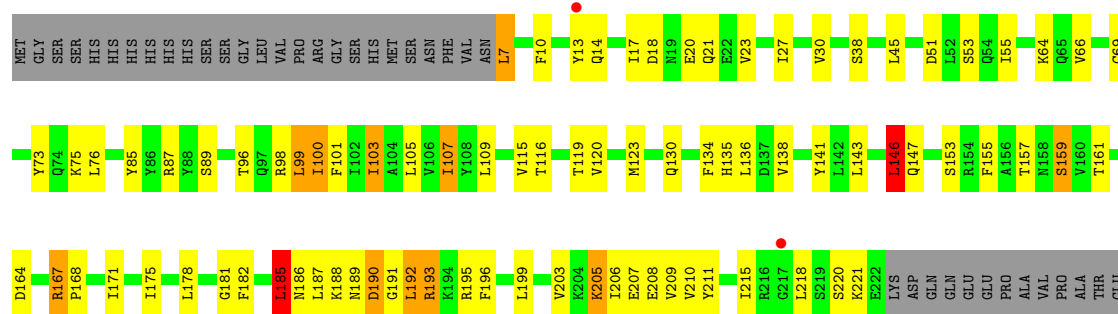




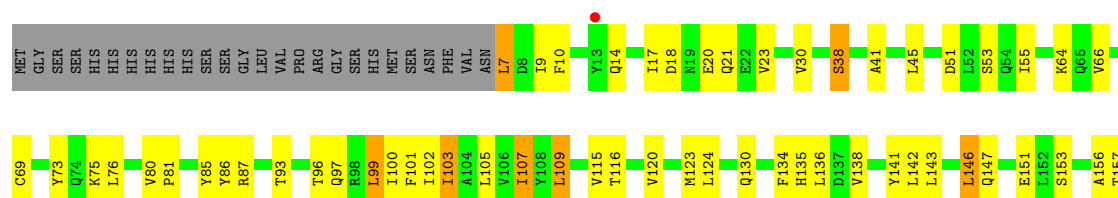
- Molecule 1: GM27569p



- Molecule 1: GM27569p



- Molecule 1: GM27569p

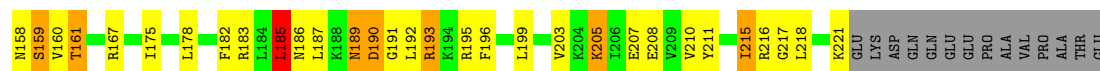
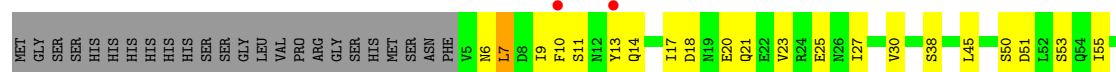




• Molecule 1: GM27569p



• Molecule 1: GM27569p



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.05Å 131.20Å 96.40Å 90.00° 98.46° 90.00°	Depositor
Resolution (Å)	48.15 – 4.20 48.15 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.15-4.20) 99.3 (48.15-4.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.237 , 0.292 0.225 , 0.283	Depositor DCC
R_{free} test set	831 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	121.6	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 127.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13931	wwPDB-VP
Average B, all atoms (Å ²)	183.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [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	0.71	0/1755	0.94	1/2367 (0.0%)
1	B	0.68	0/1759	0.94	1/2372 (0.0%)
1	C	0.67	0/1755	0.93	2/2367 (0.1%)
1	D	0.59	0/1767	0.87	1/2383 (0.0%)
1	E	0.60	0/1785	0.92	3/2406 (0.1%)
1	F	0.63	0/1776	0.92	1/2394 (0.0%)
1	G	0.69	0/1767	0.94	2/2383 (0.1%)
1	H	0.69	0/1791	0.93	1/2415 (0.0%)
All	All	0.66	0/14155	0.92	12/19087 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	216	ARG	N-CA-C	-6.75	103.11	112.30
1	E	218	LEU	N-CA-C	6.66	120.69	110.36
1	E	146	LEU	N-CA-C	-6.66	105.31	113.50
1	C	216	ARG	N-CA-C	-6.44	103.42	113.02
1	G	146	LEU	N-CA-C	-6.29	105.76	113.50
1	F	220	SER	N-CA-C	5.92	118.50	111.33
1	H	146	LEU	N-CA-C	-5.66	106.54	113.50
1	E	215	ILE	N-CA-C	-5.64	107.48	112.90
1	A	146	LEU	N-CA-C	-5.49	106.43	113.23
1	C	215	ILE	N-CA-C	-5.46	107.66	112.90
1	D	146	LEU	N-CA-C	-5.25	106.72	113.23
1	B	215	ILE	N-CA-C	-5.15	107.96	112.90

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	1727	0	1751	62	0
1	B	1731	0	1750	61	1
1	C	1727	0	1751	50	1
1	D	1739	0	1761	49	0
1	E	1757	0	1780	51	0
1	F	1748	0	1774	54	0
1	G	1739	0	1761	71	0
1	H	1763	0	1789	76	0
All	All	13931	0	14117	395	1

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 14.

All (395) 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:E:100:ILE:HD13	1:E:141:TYR:HA	1.46	0.97
1:G:100:ILE:HD13	1:G:141:TYR:HA	1.49	0.95
1:E:21:GLN:HE22	1:F:188:LYS:H	1.15	0.93
1:A:183:ARG:HB3	1:G:43:ILE:HG12	1.48	0.93
1:C:100:ILE:HD13	1:C:141:TYR:HA	1.50	0.91
1:D:100:ILE:HD13	1:D:141:TYR:HA	1.52	0.91
1:H:100:ILE:HD13	1:H:141:TYR:HA	1.52	0.90
1:A:100:ILE:HD13	1:A:141:TYR:HA	1.53	0.89
1:F:100:ILE:HD13	1:F:141:TYR:HA	1.53	0.88
1:B:100:ILE:HD13	1:B:141:TYR:HA	1.54	0.88
1:A:188:LYS:H	1:B:21:GLN:HE22	1.23	0.86
1:C:45:LEU:HD13	1:C:105:LEU:HD23	1.58	0.85
1:F:45:LEU:HD13	1:F:105:LEU:HD23	1.60	0.84
1:G:142:LEU:HD22	1:H:13:TYR:CE2	2.13	0.83
1:C:100:ILE:HD11	1:C:136:LEU:HD11	1.60	0.83
1:G:73:TYR:HH	1:G:96:THR:HG1	1.22	0.83
1:E:45:LEU:HD13	1:E:105:LEU:HD23	1.61	0.82
1:B:207:GLU:OE2	1:D:154:ARG:NH2	2.13	0.82
1:B:100:ILE:HD11	1:B:136:LEU:HD11	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD13	1:B:105:LEU:HD23	1.61	0.81
1:G:100:ILE:HD11	1:G:136:LEU:HD11	1.64	0.80
1:A:100:ILE:HD11	1:A:136:LEU:HD11	1.63	0.79
1:C:13:TYR:HD2	1:D:185:LEU:HD21	1.48	0.79
1:H:45:LEU:HD13	1:H:105:LEU:HD23	1.63	0.79
1:G:45:LEU:HD13	1:G:105:LEU:HD23	1.65	0.78
1:A:45:LEU:HD13	1:A:105:LEU:HD23	1.65	0.78
1:A:154:ARG:NH2	1:C:207:GLU:OE2	2.12	0.78
1:F:100:ILE:HD11	1:F:136:LEU:HD11	1.65	0.77
1:H:100:ILE:HD11	1:H:136:LEU:HD11	1.66	0.77
1:A:73:TYR:HH	1:A:96:THR:HG1	1.33	0.77
1:F:183:ARG:NH1	1:H:50:SER:HB2	1.98	0.77
1:E:100:ILE:HD11	1:E:136:LEU:HD11	1.67	0.76
1:B:43:ILE:HG23	1:H:183:ARG:HD2	1.67	0.76
1:D:45:LEU:HD13	1:D:105:LEU:HD23	1.69	0.75
1:D:73:TYR:HH	1:D:96:THR:HG1	1.35	0.73
1:D:100:ILE:HD11	1:D:136:LEU:HD11	1.71	0.73
1:A:66:VAL:HG11	1:A:103:ILE:HD11	1.69	0.73
1:C:73:TYR:HH	1:C:96:THR:HG1	1.34	0.72
1:G:66:VAL:HG11	1:G:103:ILE:HD11	1.71	0.72
1:B:73:TYR:HH	1:B:96:THR:HG1	1.38	0.72
1:B:66:VAL:HG11	1:B:103:ILE:HD11	1.72	0.72
1:E:73:TYR:HH	1:E:96:THR:HG1	1.37	0.70
1:C:51:ASP:OD1	1:C:53:SER:OG	2.10	0.69
1:F:200:LYS:HB2	1:H:161:THR:HG21	1.74	0.69
1:B:39:LYS:NZ	1:H:193:ARG:HH12	1.91	0.69
1:B:43:ILE:HG12	1:H:183:ARG:HD3	1.76	0.66
1:D:51:ASP:OD1	1:D:53:SER:OG	2.13	0.66
1:A:39:LYS:HE3	1:C:186:ASN:OD1	1.96	0.66
1:B:39:LYS:NZ	1:H:193:ARG:NH1	2.44	0.66
1:G:188:LYS:O	1:H:21:GLN:NE2	2.29	0.65
1:H:6:ASN:OD1	1:H:7:LEU:N	2.29	0.65
1:D:66:VAL:HG11	1:D:103:ILE:HD11	1.77	0.65
1:A:51:ASP:OD1	1:A:53:SER:OG	2.14	0.65
1:F:204:LYS:HD3	1:H:161:THR:HA	1.79	0.65
1:G:187:LEU:HB3	1:G:193:ARG:HG2	1.78	0.65
1:A:182:PHE:CE1	1:B:10:PHE:HE2	2.15	0.64
1:F:66:VAL:HG11	1:F:103:ILE:HD11	1.79	0.64
1:E:66:VAL:HG11	1:E:103:ILE:HD11	1.79	0.64
1:B:51:ASP:OD1	1:B:53:SER:OG	2.14	0.63
1:E:51:ASP:OD1	1:E:53:SER:OG	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ILE:HG12	1:D:120:VAL:HG11	1.81	0.63
1:H:66:VAL:HG11	1:H:103:ILE:HD11	1.80	0.63
1:G:142:LEU:HD22	1:H:13:TYR:HE2	1.60	0.62
1:H:51:ASP:OD1	1:H:53:SER:OG	2.16	0.61
1:F:73:TYR:HH	1:F:96:THR:HG1	1.41	0.61
1:C:130:GLN:NE2	1:D:87:ARG:HH11	1.99	0.61
1:F:51:ASP:OD1	1:F:53:SER:OG	2.16	0.61
1:G:51:ASP:OD1	1:G:53:SER:OG	2.18	0.61
1:G:182:PHE:CE1	1:H:10:PHE:HE2	2.19	0.60
1:E:21:GLN:NE2	1:F:188:LYS:H	1.93	0.60
1:A:7:LEU:N	1:A:9:ILE:HD12	2.16	0.60
1:C:66:VAL:HG11	1:C:103:ILE:HD11	1.83	0.60
1:G:184:LEU:HD21	1:H:11:SER:HB3	1.84	0.60
1:H:143:LEU:HD22	1:H:195:ARG:HD2	1.84	0.60
1:B:39:LYS:HZ1	1:H:193:ARG:NH1	2.00	0.59
1:A:211:TYR:OH	1:G:212:ASP:OD2	2.16	0.59
1:F:100:ILE:HG12	1:F:120:VAL:HG11	1.86	0.58
1:B:100:ILE:HG12	1:B:120:VAL:HG11	1.84	0.58
1:A:100:ILE:HG12	1:A:120:VAL:HG11	1.86	0.57
1:C:100:ILE:HG12	1:C:120:VAL:HG11	1.86	0.57
1:F:7:LEU:N	1:F:9:ILE:HD12	2.19	0.57
1:H:6:ASN:HB3	1:H:9:ILE:HD11	1.87	0.57
1:G:182:PHE:O	1:G:185:LEU:HB2	2.04	0.57
1:E:100:ILE:HG12	1:E:120:VAL:HG11	1.87	0.56
1:H:55:ILE:HG23	1:H:109:LEU:HD13	1.87	0.56
1:A:183:ARG:CB	1:G:43:ILE:HG12	2.29	0.56
1:A:85:TYR:HE1	1:A:134:PHE:CE2	2.23	0.56
1:F:200:LYS:HE3	1:H:158:ASN:OD1	2.06	0.55
1:C:10:PHE:HE2	1:D:182:PHE:CD1	2.25	0.55
1:A:210:VAL:HG12	1:G:161:THR:OG1	2.07	0.55
1:A:130:GLN:HB3	1:A:135:HIS:CE1	2.41	0.55
1:C:187:LEU:HB3	1:C:193:ARG:HG2	1.89	0.54
1:B:85:TYR:HE1	1:B:134:PHE:CE2	2.25	0.54
1:E:220:SER:O	1:E:221:LYS:HB3	2.07	0.54
1:E:14:GLN:NE2	1:E:18:ASP:OD1	2.40	0.54
1:E:7:LEU:HD13	1:E:7:LEU:O	2.07	0.54
1:E:182:PHE:HB3	1:E:196:PHE:CE1	2.42	0.54
1:H:14:GLN:NE2	1:H:18:ASP:OD1	2.41	0.54
1:A:143:LEU:HD22	1:A:195:ARG:HD2	1.90	0.53
1:C:203:VAL:O	1:C:207:GLU:HG2	2.08	0.53
1:G:85:TYR:HE1	1:G:134:PHE:CE2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ILE:HG12	1:G:120:VAL:HG11	1.89	0.53
1:A:188:LYS:NZ	1:B:25:GLU:OE2	2.32	0.53
1:E:107:ILE:HG21	1:E:115:VAL:HB	1.90	0.53
1:G:165:TYR:CD2	1:G:218:LEU:HB3	2.43	0.53
1:A:14:GLN:NE2	1:A:18:ASP:OD1	2.43	0.52
1:B:187:LEU:HB3	1:B:193:ARG:HG2	1.90	0.52
1:C:86:TYR:CE2	1:D:87:ARG:HD2	2.45	0.52
1:F:187:LEU:HB3	1:F:193:ARG:HG2	1.90	0.52
1:H:100:ILE:HG12	1:H:120:VAL:HG11	1.89	0.52
1:H:155:PHE:O	1:H:159:SER:HB2	2.10	0.52
1:F:107:ILE:HG21	1:F:115:VAL:HB	1.91	0.52
1:G:130:GLN:HB3	1:G:135:HIS:CE1	2.44	0.52
1:G:185:LEU:HA	1:H:14:GLN:HB2	1.90	0.52
1:E:13:TYR:HD2	1:F:185:LEU:HD21	1.73	0.52
1:E:85:TYR:HE1	1:E:134:PHE:CE2	2.27	0.52
1:F:183:ARG:HH12	1:H:50:SER:HB2	1.71	0.52
1:C:107:ILE:HG21	1:C:115:VAL:HB	1.92	0.51
1:A:185:LEU:HD21	1:B:13:TYR:HD2	1.75	0.51
1:F:203:VAL:O	1:F:207:GLU:HG2	2.10	0.51
1:G:142:LEU:HB2	1:H:13:TYR:OH	2.10	0.51
1:H:130:GLN:HB3	1:H:135:HIS:CE1	2.45	0.51
1:H:182:PHE:HB3	1:H:196:PHE:CE1	2.45	0.51
1:B:107:ILE:HG21	1:B:115:VAL:HB	1.92	0.51
1:B:157:THR:O	1:H:211:TYR:HD1	1.94	0.51
1:D:143:LEU:HD22	1:D:195:ARG:HD2	1.93	0.51
1:F:14:GLN:NE2	1:F:18:ASP:OD1	2.44	0.50
1:A:142:LEU:HD22	1:B:13:TYR:CE2	2.47	0.50
1:D:182:PHE:HB3	1:D:196:PHE:CE1	2.47	0.50
1:F:143:LEU:HD22	1:F:195:ARG:HD2	1.93	0.50
1:G:14:GLN:NE2	1:G:18:ASP:OD1	2.44	0.50
1:B:143:LEU:HD22	1:B:195:ARG:HD2	1.93	0.50
1:A:30:VAL:HG11	1:A:76:LEU:HB2	1.94	0.50
1:H:85:TYR:HE1	1:H:134:PHE:CE2	2.30	0.50
1:G:190:ASP:OD2	1:H:21:GLN:NE2	2.45	0.49
1:H:187:LEU:HB3	1:H:193:ARG:HG2	1.93	0.49
1:H:30:VAL:HG11	1:H:76:LEU:HB2	1.93	0.49
1:G:20:GLU:HG3	1:G:87:ARG:HH21	1.77	0.49
1:D:187:LEU:HB3	1:D:193:ARG:HG2	1.94	0.49
1:E:155:PHE:O	1:E:159:SER:HB2	2.12	0.49
1:H:62:ALA:O	1:H:65:GLN:HB2	2.13	0.49
1:E:203:VAL:O	1:E:207:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:HG23	1:H:183:ARG:CD	2.41	0.49
1:D:119:THR:O	1:D:123:MET:HG3	2.13	0.49
1:E:146:LEU:HG	1:E:182:PHE:CZ	2.48	0.49
1:G:203:VAL:O	1:G:207:GLU:HG2	2.12	0.49
1:G:182:PHE:HB3	1:G:196:PHE:CE1	2.48	0.49
1:E:187:LEU:HB3	1:E:193:ARG:HG2	1.95	0.48
1:H:203:VAL:O	1:H:207:GLU:HG2	2.14	0.48
1:A:87:ARG:HH11	1:B:130:GLN:NE2	2.11	0.48
1:B:203:VAL:O	1:B:207:GLU:HG2	2.13	0.48
1:F:182:PHE:HB3	1:F:196:PHE:CE1	2.48	0.48
1:H:7:LEU:HD13	1:H:7:LEU:O	2.13	0.48
1:H:107:ILE:HG21	1:H:115:VAL:HB	1.94	0.48
1:G:30:VAL:HG11	1:G:76:LEU:HB2	1.95	0.48
1:E:119:THR:O	1:E:123:MET:HG3	2.14	0.48
1:A:182:PHE:HB3	1:A:196:PHE:CE1	2.49	0.48
1:F:116:THR:O	1:F:120:VAL:HG23	2.14	0.48
1:G:142:LEU:HB2	1:H:13:TYR:CZ	2.49	0.48
1:G:143:LEU:HD22	1:G:195:ARG:HD2	1.95	0.48
1:B:182:PHE:HB3	1:B:196:PHE:CE1	2.48	0.48
1:C:10:PHE:HD2	1:D:181:GLY:O	1.96	0.48
1:A:55:ILE:HG23	1:A:109:LEU:HD13	1.96	0.48
1:E:55:ILE:HG23	1:E:109:LEU:HD13	1.96	0.48
1:E:101:PHE:HB2	1:E:147:GLN:HB2	1.95	0.48
1:A:187:LEU:HB3	1:A:193:ARG:HG2	1.95	0.47
1:G:186:ASN:HB2	1:H:14:GLN:NE2	2.29	0.47
1:B:119:THR:O	1:B:123:MET:HG3	2.14	0.47
1:C:182:PHE:HB3	1:C:196:PHE:CE1	2.49	0.47
1:D:55:ILE:HG23	1:D:109:LEU:HD13	1.95	0.47
1:F:85:TYR:HE1	1:F:134:PHE:CE2	2.32	0.47
1:C:30:VAL:HG11	1:C:76:LEU:HB2	1.96	0.47
1:F:130:GLN:HB3	1:F:135:HIS:CE1	2.50	0.47
1:G:185:LEU:HD22	1:H:14:GLN:HB2	1.95	0.47
1:C:143:LEU:HD22	1:C:195:ARG:HD2	1.97	0.47
1:D:30:VAL:HG11	1:D:76:LEU:HB2	1.96	0.47
1:F:30:VAL:HG11	1:F:76:LEU:HB2	1.96	0.47
1:C:123:MET:HE2	1:C:123:MET:HB3	1.83	0.47
1:D:107:ILE:HG21	1:D:115:VAL:HB	1.95	0.47
1:E:30:VAL:HG11	1:E:76:LEU:HB2	1.97	0.47
1:F:73:TYR:OH	1:F:96:THR:OG1	2.25	0.47
1:G:213:VAL:HG12	1:G:218:LEU:HD12	1.97	0.47
1:C:85:TYR:HE1	1:C:134:PHE:CE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LYS:HB3	1:C:205:LYS:HE2	1.58	0.47
1:G:87:ARG:HD2	1:H:86:TYR:CZ	2.49	0.47
1:A:146:LEU:HG	1:A:182:PHE:CZ	2.50	0.47
1:A:164:ASP:OD2	1:A:167:ARG:HD2	2.15	0.47
1:E:143:LEU:HD22	1:E:195:ARG:HD2	1.97	0.47
1:G:38:SER:HB2	1:G:99:LEU:CD2	2.45	0.47
1:C:13:TYR:CD2	1:D:185:LEU:HD21	2.39	0.46
1:C:14:GLN:NE2	1:C:18:ASP:OD1	2.48	0.46
1:E:87:ARG:HD2	1:F:86:TYR:CZ	2.50	0.46
1:B:14:GLN:NE2	1:B:18:ASP:OD1	2.48	0.46
1:C:130:GLN:HB3	1:C:135:HIS:CE1	2.50	0.46
1:E:208:GLU:O	1:E:211:TYR:HB3	2.16	0.46
1:F:64:LYS:HA	1:F:64:LYS:HD3	1.80	0.46
1:A:107:ILE:HG21	1:A:115:VAL:HB	1.98	0.46
1:B:116:THR:O	1:B:120:VAL:HG23	2.15	0.46
1:D:14:GLN:NE2	1:D:18:ASP:OD1	2.48	0.46
1:D:156:ALA:O	1:D:160:VAL:HG23	2.16	0.46
1:A:203:VAL:O	1:A:207:GLU:HG2	2.14	0.46
1:C:156:ALA:HB2	1:C:171:ILE:HD12	1.97	0.46
1:G:185:LEU:C	1:H:14:GLN:CD	2.84	0.46
1:H:73:TYR:OH	1:H:96:THR:OG1	2.08	0.46
1:B:130:GLN:HB3	1:B:135:HIS:CE1	2.50	0.46
1:G:192:LEU:O	1:G:192:LEU:HD12	2.16	0.46
1:C:84:GLN:NE2	1:D:130:GLN:NE2	2.64	0.46
1:G:13:TYR:HE1	1:H:138:VAL:HG13	1.80	0.46
1:E:116:THR:O	1:E:120:VAL:HG23	2.16	0.46
1:F:101:PHE:HB2	1:F:147:GLN:HB2	1.98	0.46
1:G:107:ILE:HG21	1:G:115:VAL:HB	1.97	0.46
1:D:85:TYR:HE1	1:D:134:PHE:CE2	2.34	0.46
1:C:55:ILE:HG23	1:C:109:LEU:HD13	1.98	0.45
1:B:30:VAL:HG11	1:B:76:LEU:HB2	1.97	0.45
1:D:130:GLN:HB3	1:D:135:HIS:CE1	2.50	0.45
1:G:188:LYS:HD3	1:H:25:GLU:OE2	2.16	0.45
1:B:20:GLU:HG3	1:B:87:ARG:HH21	1.82	0.45
1:C:10:PHE:HE2	1:D:182:PHE:CE1	2.34	0.45
1:G:41:ALA:HB3	1:G:102:ILE:HD13	1.99	0.45
1:A:155:PHE:O	1:A:159:SER:HB2	2.16	0.45
1:A:182:PHE:O	1:A:185:LEU:HB2	2.16	0.45
1:D:105:LEU:HD13	1:D:151:GLU:HG2	1.99	0.45
1:G:86:TYR:CZ	1:H:87:ARG:HD2	2.52	0.45
1:G:116:THR:O	1:G:120:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLN:HE22	1:D:87:ARG:HH11	1.61	0.45
1:E:13:TYR:CE2	1:F:142:LEU:HD22	2.51	0.45
1:F:156:ALA:O	1:F:160:VAL:HG23	2.16	0.45
1:G:205:LYS:HE2	1:G:205:LYS:HB3	1.66	0.45
1:B:55:ILE:HG23	1:B:109:LEU:HD13	1.98	0.45
1:B:185:LEU:HB3	1:B:186:ASN:H	1.46	0.45
1:E:69:CYS:SG	1:E:99:LEU:HD11	2.57	0.45
1:A:205:LYS:HB3	1:A:205:LYS:HE2	1.64	0.45
1:G:139:GLU:OE2	1:H:20:GLU:OE1	2.35	0.45
1:G:146:LEU:HG	1:G:182:PHE:CZ	2.52	0.45
1:G:213:VAL:HA	1:G:218:LEU:HD12	1.99	0.45
1:A:64:LYS:HD3	1:A:64:LYS:HA	1.70	0.44
1:B:80:VAL:HA	1:B:81:PRO:HD3	1.84	0.44
1:D:64:LYS:HA	1:D:64:LYS:HD3	1.77	0.44
1:E:199:LEU:O	1:E:203:VAL:HG23	2.17	0.44
1:B:182:PHE:O	1:B:185:LEU:HB2	2.17	0.44
1:B:205:LYS:HB3	1:B:205:LYS:HE2	1.63	0.44
1:D:69:CYS:SG	1:D:99:LEU:HD11	2.57	0.44
1:G:185:LEU:CD2	1:H:14:GLN:HB2	2.47	0.44
1:B:52:LEU:HD23	1:B:55:ILE:HD11	1.98	0.44
1:B:64:LYS:HA	1:B:64:LYS:HD3	1.77	0.44
1:E:182:PHE:O	1:E:185:LEU:HB2	2.18	0.44
1:G:190:ASP:HB2	1:G:191:GLY:H	1.59	0.44
1:F:156:ALA:HB2	1:F:171:ILE:HD12	2.00	0.44
1:A:116:THR:O	1:A:120:VAL:HG23	2.17	0.44
1:A:156:ALA:O	1:A:160:VAL:HG23	2.17	0.44
1:D:155:PHE:O	1:D:159:SER:HB2	2.17	0.44
1:F:103:ILE:HD13	1:F:123:MET:SD	2.58	0.44
1:G:185:LEU:HD22	1:H:14:GLN:OE1	2.18	0.44
1:A:101:PHE:HB2	1:A:147:GLN:HB2	2.00	0.44
1:F:208:GLU:O	1:F:211:TYR:HB3	2.18	0.44
1:H:146:LEU:HG	1:H:182:PHE:CZ	2.53	0.44
1:A:86:TYR:CZ	1:B:87:ARG:HD2	2.53	0.44
1:B:146:LEU:HG	1:B:182:PHE:CZ	2.52	0.44
1:C:41:ALA:HB3	1:C:102:ILE:HD13	2.00	0.44
1:E:181:GLY:O	1:F:10:PHE:HD2	2.01	0.44
1:F:38:SER:HB2	1:F:99:LEU:CD2	2.48	0.44
1:A:105:LEU:HD13	1:A:151:GLU:HG2	2.00	0.43
1:E:130:GLN:HB3	1:E:135:HIS:CE1	2.52	0.43
1:G:155:PHE:O	1:G:159:SER:HB2	2.18	0.43
1:H:103:ILE:HD13	1:H:123:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLU:HG3	1:A:87:ARG:HH21	1.82	0.43
1:G:182:PHE:HE1	1:H:10:PHE:HE2	1.63	0.43
1:H:105:LEU:HD13	1:H:151:GLU:HG2	2.00	0.43
1:A:143:LEU:HD21	1:A:192:LEU:HB2	2.00	0.43
1:B:156:ALA:O	1:B:160:VAL:HG23	2.19	0.43
1:G:142:LEU:HD13	1:H:13:TYR:CE2	2.53	0.43
1:G:146:LEU:HD23	1:G:146:LEU:HA	1.61	0.43
1:G:123:MET:HE2	1:G:123:MET:HB3	1.87	0.43
1:B:155:PHE:O	1:B:159:SER:HB2	2.18	0.43
1:E:146:LEU:HA	1:E:146:LEU:HD23	1.65	0.43
1:G:55:ILE:HG23	1:G:109:LEU:HD13	1.99	0.43
1:A:7:LEU:HD21	1:B:184:LEU:HD22	2.01	0.43
1:A:142:LEU:HD22	1:B:13:TYR:CZ	2.53	0.43
1:D:80:VAL:HA	1:D:81:PRO:HD3	1.83	0.43
1:F:105:LEU:HD13	1:F:151:GLU:HG2	2.00	0.43
1:D:101:PHE:HB2	1:D:147:GLN:HB2	2.00	0.43
1:E:64:LYS:HD3	1:E:64:LYS:HA	1.78	0.43
1:F:182:PHE:O	1:F:185:LEU:HB2	2.18	0.43
1:C:101:PHE:HB2	1:C:147:GLN:HB2	2.00	0.43
1:C:119:THR:O	1:C:123:MET:HG3	2.19	0.43
1:D:199:LEU:O	1:D:203:VAL:HG23	2.19	0.43
1:G:175:ILE:HD13	1:G:175:ILE:HA	1.89	0.43
1:A:80:VAL:HA	1:A:81:PRO:HD3	1.86	0.43
1:F:55:ILE:HG23	1:F:109:LEU:HD13	1.99	0.43
1:H:101:PHE:HB2	1:H:147:GLN:HB2	1.99	0.43
1:C:84:GLN:HG2	1:D:130:GLN:HE22	1.83	0.43
1:C:190:ASP:HB2	1:C:191:GLY:H	1.59	0.43
1:E:205:LYS:HB3	1:E:205:LYS:HE2	1.75	0.43
1:G:64:LYS:HA	1:G:64:LYS:HD3	1.73	0.43
1:G:105:LEU:HD13	1:G:151:GLU:HG2	2.01	0.43
1:G:117:ARG:CZ	1:G:138:VAL:HG23	2.48	0.43
1:A:87:ARG:HH11	1:B:130:GLN:HE22	1.67	0.42
1:B:43:ILE:O	1:B:46:GLN:HB2	2.18	0.42
1:C:155:PHE:O	1:C:159:SER:HB2	2.19	0.42
1:D:41:ALA:HB3	1:D:102:ILE:HD13	2.00	0.42
1:H:190:ASP:HB2	1:H:191:GLY:H	1.63	0.42
1:B:101:PHE:HB2	1:B:147:GLN:HB2	2.01	0.42
1:C:13:TYR:CE2	1:D:185:LEU:HD11	2.54	0.42
1:E:10:PHE:HE2	1:F:182:PHE:CE1	2.37	0.42
1:G:85:TYR:CE1	1:G:134:PHE:CE2	3.07	0.42
1:G:119:THR:O	1:G:123:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:LEU:HD22	1:H:14:GLN:CA	2.50	0.42
1:H:189:ASN:HA	1:H:193:ARG:HG3	2.00	0.42
1:A:190:ASP:HB2	1:A:191:GLY:H	1.63	0.42
1:D:205:LYS:HB3	1:D:205:LYS:HE2	1.71	0.42
1:E:221:LYS:HB3	1:E:221:LYS:HE3	1.85	0.42
1:A:138:VAL:HG11	1:B:16:TYR:CE2	2.54	0.42
1:A:208:GLU:O	1:A:211:TYR:HB3	2.20	0.42
1:A:73:TYR:OH	1:A:96:THR:OG1	2.14	0.42
1:A:87:ARG:HD2	1:B:86:TYR:CE2	2.55	0.42
1:C:199:LEU:O	1:C:203:VAL:HG23	2.19	0.42
1:C:218:LEU:H	1:C:218:LEU:HG	1.60	0.42
1:D:143:LEU:HD21	1:D:192:LEU:HB2	2.02	0.42
1:H:64:LYS:HD3	1:H:64:LYS:HA	1.73	0.42
1:H:208:GLU:O	1:H:211:TYR:HB3	2.19	0.42
1:D:62:ALA:O	1:D:65:GLN:HB2	2.19	0.42
1:D:203:VAL:O	1:D:207:GLU:HG2	2.20	0.42
1:G:103:ILE:HD13	1:G:123:MET:SD	2.60	0.42
1:G:185:LEU:O	1:G:186:ASN:ND2	2.53	0.42
1:A:17:ILE:HG23	1:A:21:GLN:OE1	2.20	0.42
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.91	0.42
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.67	0.42
1:B:157:THR:HG23	1:H:211:TYR:CD1	2.55	0.42
1:C:10:PHE:CD2	1:D:181:GLY:C	2.98	0.42
1:D:146:LEU:HD23	1:D:146:LEU:HA	1.65	0.42
1:D:185:LEU:O	1:D:186:ASN:ND2	2.52	0.42
1:H:199:LEU:O	1:H:203:VAL:HG23	2.20	0.42
1:C:164:ASP:OD2	1:C:167:ARG:HB2	2.20	0.42
1:D:190:ASP:HB2	1:D:191:GLY:H	1.62	0.42
1:F:143:LEU:HD21	1:F:192:LEU:HB2	2.02	0.42
1:H:216:ARG:HA	1:H:217:GLY:HA3	1.51	0.42
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.67	0.41
1:B:167:ARG:HB3	1:B:168:PRO:HD3	2.02	0.41
1:F:69:CYS:SG	1:F:99:LEU:HD11	2.59	0.41
1:H:175:ILE:HD13	1:H:175:ILE:HA	1.93	0.41
1:F:123:MET:HE2	1:F:123:MET:HB3	1.95	0.41
1:A:43:ILE:O	1:A:46:GLN:HB2	2.20	0.41
1:F:120:VAL:O	1:F:124:LEU:HD12	2.20	0.41
1:F:146:LEU:HD23	1:F:146:LEU:HA	1.64	0.41
1:A:130:GLN:NE2	1:B:84:GLN:NE2	2.68	0.41
1:A:185:LEU:HD22	1:B:14:GLN:OE1	2.20	0.41
1:E:143:LEU:HD21	1:E:192:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:LYS:HB2	1:F:21:GLN:NE2	2.35	0.41
1:G:101:PHE:HB2	1:G:147:GLN:HB2	2.02	0.41
1:A:216:ARG:HG2	1:G:216:ARG:NH2	2.35	0.41
1:H:182:PHE:O	1:H:185:LEU:HB2	2.21	0.41
1:B:105:LEU:HD13	1:B:151:GLU:HG2	2.01	0.41
1:E:20:GLU:HG3	1:E:87:ARG:HH21	1.85	0.41
1:E:175:ILE:HD13	1:E:175:ILE:HA	1.93	0.41
1:H:123:MET:HB3	1:H:123:MET:HE2	1.82	0.41
1:B:171:ILE:HG22	1:B:206:ILE:HG21	2.02	0.41
1:C:185:LEU:O	1:C:186:ASN:ND2	2.49	0.41
1:F:146:LEU:HG	1:F:182:PHE:CZ	2.55	0.41
1:C:25:GLU:HG3	1:C:28:ARG:HH12	1.85	0.41
1:E:190:ASP:HB2	1:E:191:GLY:H	1.64	0.41
1:F:107:ILE:HD12	1:F:107:ILE:HA	1.79	0.41
1:A:69:CYS:SG	1:A:99:LEU:HD11	2.60	0.41
1:A:179:ASN:OD1	1:A:199:LEU:HD23	2.21	0.41
1:C:164:ASP:OD2	1:C:167:ARG:HD2	2.21	0.41
1:G:208:GLU:O	1:G:211:TYR:HB3	2.21	0.41
1:H:117:ARG:CZ	1:H:138:VAL:HG23	2.51	0.41
1:H:215:ILE:HD12	1:H:215:ILE:HA	1.87	0.41
1:B:107:ILE:HD12	1:B:107:ILE:HA	1.79	0.41
1:C:116:THR:O	1:C:120:VAL:HG23	2.21	0.41
1:C:212:ASP:O	1:C:215:ILE:HG22	2.21	0.41
1:D:182:PHE:O	1:D:185:LEU:HB2	2.21	0.41
1:E:181:GLY:O	1:F:10:PHE:CD2	2.74	0.41
1:C:105:LEU:HD13	1:C:151:GLU:HG2	2.03	0.40
1:D:146:LEU:HG	1:D:182:PHE:CZ	2.55	0.40
1:H:146:LEU:HA	1:H:146:LEU:HD23	1.65	0.40
1:B:190:ASP:OD1	1:B:190:ASP:N	2.54	0.40
1:C:182:PHE:O	1:C:185:LEU:HB2	2.22	0.40
1:D:116:THR:O	1:D:120:VAL:HG23	2.21	0.40
1:E:164:ASP:OD2	1:E:167:ARG:HD2	2.21	0.40
1:E:171:ILE:HG22	1:E:206:ILE:HG21	2.04	0.40
1:F:20:GLU:HG3	1:F:87:ARG:HH21	1.87	0.40
1:A:171:ILE:HG22	1:A:206:ILE:HG21	2.04	0.40
1:E:85:TYR:CE1	1:E:134:PHE:CE2	3.09	0.40
1:E:123:MET:HE2	1:E:123:MET:HB3	1.89	0.40
1:E:192:LEU:O	1:E:192:LEU:HD12	2.21	0.40
1:G:199:LEU:O	1:G:203:VAL:HG23	2.22	0.40
1:H:156:ALA:O	1:H:160:VAL:HG23	2.22	0.40
1:C:20:GLU:HG3	1:C:87:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ALA:HB3	1:F:102:ILE:HD13	2.03	0.40
1:F:80:VAL:HA	1:F:81:PRO:HD3	1.87	0.40
1:B:190:ASP:HB2	1:B:191:GLY:H	1.58	0.40
1:E:168:PRO:HB3	1:E:209:VAL:HG12	2.03	0.40
1:F:93:THR:O	1:F:97:GLN:HG3	2.21	0.40
1:G:182:PHE:CE1	1:H:10:PHE:CE2	3.06	0.40
1:H:205:LYS:HB3	1:H:205:LYS:HE2	1.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LYS:NZ	1:C:132:GLU:O[2_645]	1.92	0.28

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	210/255 (82%)	193 (92%)	13 (6%)	4 (2%)	6	32
1	B	211/255 (83%)	193 (92%)	14 (7%)	4 (2%)	6	32
1	C	210/255 (82%)	193 (92%)	14 (7%)	3 (1%)	9	39
1	D	212/255 (83%)	195 (92%)	14 (7%)	3 (1%)	9	39
1	E	214/255 (84%)	193 (90%)	18 (8%)	3 (1%)	9	39
1	F	213/255 (84%)	195 (92%)	14 (7%)	4 (2%)	6	32
1	G	212/255 (83%)	191 (90%)	18 (8%)	3 (1%)	9	39
1	H	215/255 (84%)	197 (92%)	14 (6%)	4 (2%)	6	32
All	All	1697/2040 (83%)	1550 (91%)	119 (7%)	28 (2%)	7	37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	LEU
1	A	186	ASN
1	A	189	ASN
1	B	185	LEU
1	B	186	ASN
1	B	189	ASN
1	C	185	LEU
1	C	186	ASN
1	C	189	ASN
1	D	185	LEU
1	D	186	ASN
1	D	189	ASN
1	E	185	LEU
1	E	186	ASN
1	E	189	ASN
1	F	185	LEU
1	F	186	ASN
1	F	189	ASN
1	G	185	LEU
1	G	186	ASN
1	H	185	LEU
1	H	186	ASN
1	H	189	ASN
1	G	189	ASN
1	B	217	GLY
1	F	217	GLY
1	A	145	ILE
1	H	145	ILE

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	188/226 (83%)	163 (87%)	25 (13%)	4	17
1	B	189/226 (84%)	167 (88%)	22 (12%)	5	20
1	C	188/226 (83%)	162 (86%)	26 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	190/226 (84%)	167 (88%)	23 (12%)	5	19
1	E	192/226 (85%)	166 (86%)	26 (14%)	4	17
1	F	191/226 (84%)	169 (88%)	22 (12%)	5	20
1	G	190/226 (84%)	166 (87%)	24 (13%)	4	18
1	H	193/226 (85%)	166 (86%)	27 (14%)	3	16
All	All	1521/1808 (84%)	1326 (87%)	195 (13%)	4	18

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	ILE
1	A	23	VAL
1	A	27	ILE
1	A	38	SER
1	A	75	LYS
1	A	89	SER
1	A	96	THR
1	A	98	ARG
1	A	99	LEU
1	A	103	ILE
1	A	107	ILE
1	A	138	VAL
1	A	146	LEU
1	A	157	THR
1	A	159	SER
1	A	161	THR
1	A	167	ARG
1	A	178	LEU
1	A	185	LEU
1	A	190	ASP
1	A	192	LEU
1	A	193	ARG
1	A	205	LYS
1	A	210	VAL
1	B	17	ILE
1	B	23	VAL
1	B	27	ILE
1	B	38	SER
1	B	75	LYS

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Mol	Chain	Res	Type
1	B	89	SER
1	B	98	ARG
1	B	99	LEU
1	B	103	ILE
1	B	107	ILE
1	B	138	VAL
1	B	146	LEU
1	B	157	THR
1	B	159	SER
1	B	161	THR
1	B	167	ARG
1	B	185	LEU
1	B	190	ASP
1	B	192	LEU
1	B	193	ARG
1	B	205	LYS
1	B	210	VAL
1	C	7	LEU
1	C	17	ILE
1	C	23	VAL
1	C	27	ILE
1	C	29	ILE
1	C	38	SER
1	C	75	LYS
1	C	89	SER
1	C	98	ARG
1	C	99	LEU
1	C	103	ILE
1	C	107	ILE
1	C	138	VAL
1	C	146	LEU
1	C	153	SER
1	C	157	THR
1	C	159	SER
1	C	161	THR
1	C	167	ARG
1	C	185	LEU
1	C	190	ASP
1	C	192	LEU
1	C	193	ARG
1	C	205	LYS
1	C	210	VAL

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Mol	Chain	Res	Type
1	C	218	LEU
1	D	7	LEU
1	D	17	ILE
1	D	23	VAL
1	D	27	ILE
1	D	38	SER
1	D	89	SER
1	D	99	LEU
1	D	103	ILE
1	D	107	ILE
1	D	138	VAL
1	D	146	LEU
1	D	157	THR
1	D	159	SER
1	D	161	THR
1	D	167	ARG
1	D	178	LEU
1	D	185	LEU
1	D	190	ASP
1	D	192	LEU
1	D	193	ARG
1	D	205	LYS
1	D	210	VAL
1	D	219	SER
1	E	7	LEU
1	E	17	ILE
1	E	23	VAL
1	E	27	ILE
1	E	38	SER
1	E	75	LYS
1	E	89	SER
1	E	98	ARG
1	E	99	LEU
1	E	100	ILE
1	E	103	ILE
1	E	107	ILE
1	E	138	VAL
1	E	146	LEU
1	E	153	SER
1	E	157	THR
1	E	159	SER
1	E	161	THR

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Mol	Chain	Res	Type
1	E	167	ARG
1	E	178	LEU
1	E	185	LEU
1	E	190	ASP
1	E	192	LEU
1	E	193	ARG
1	E	205	LYS
1	E	210	VAL
1	F	7	LEU
1	F	17	ILE
1	F	23	VAL
1	F	38	SER
1	F	75	LYS
1	F	99	LEU
1	F	103	ILE
1	F	107	ILE
1	F	109	LEU
1	F	138	VAL
1	F	146	LEU
1	F	153	SER
1	F	157	THR
1	F	159	SER
1	F	161	THR
1	F	167	ARG
1	F	185	LEU
1	F	190	ASP
1	F	192	LEU
1	F	193	ARG
1	F	205	LYS
1	F	210	VAL
1	G	17	ILE
1	G	23	VAL
1	G	27	ILE
1	G	38	SER
1	G	75	LYS
1	G	89	SER
1	G	99	LEU
1	G	100	ILE
1	G	103	ILE
1	G	107	ILE
1	G	138	VAL
1	G	146	LEU

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Mol	Chain	Res	Type
1	G	157	THR
1	G	159	SER
1	G	161	THR
1	G	167	ARG
1	G	175	ILE
1	G	185	LEU
1	G	187	LEU
1	G	190	ASP
1	G	192	LEU
1	G	193	ARG
1	G	205	LYS
1	G	210	VAL
1	H	7	LEU
1	H	17	ILE
1	H	23	VAL
1	H	27	ILE
1	H	38	SER
1	H	75	LYS
1	H	89	SER
1	H	96	THR
1	H	99	LEU
1	H	103	ILE
1	H	107	ILE
1	H	138	VAL
1	H	146	LEU
1	H	157	THR
1	H	159	SER
1	H	161	THR
1	H	167	ARG
1	H	178	LEU
1	H	185	LEU
1	H	190	ASP
1	H	192	LEU
1	H	193	ARG
1	H	205	LYS
1	H	210	VAL
1	H	215	ILE
1	H	218	LEU
1	H	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	14	GLN
1	A	65	GLN
1	A	130	GLN
1	A	170	ASN
1	B	12	ASN
1	B	21	GLN
1	B	65	GLN
1	B	130	GLN
1	B	170	ASN
1	C	14	GLN
1	C	130	GLN
1	C	170	ASN
1	D	14	GLN
1	D	130	GLN
1	D	158	ASN
1	D	170	ASN
1	E	21	GLN
1	E	65	GLN
1	F	12	ASN
1	F	170	ASN
1	G	12	ASN
1	G	65	GLN
1	G	170	ASN
1	H	65	GLN
1	H	170	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	212/255 (83%)	-0.12	4 (1%)	66	51	104, 163, 229, 309	0
1	B	213/255 (83%)	-0.26	5 (2%)	61	47	121, 178, 243, 382	0
1	C	212/255 (83%)	-0.13	4 (1%)	66	51	106, 166, 239, 431	0
1	D	214/255 (83%)	-0.19	2 (0%)	81	66	110, 182, 245, 311	0
1	E	216/255 (84%)	-0.12	2 (0%)	81	66	127, 190, 265, 439	0
1	F	215/255 (84%)	-0.18	1 (0%)	87	75	121, 178, 247, 297	0
1	G	214/255 (83%)	-0.13	3 (1%)	73	57	105, 175, 237, 329	0
1	H	217/255 (85%)	-0.04	2 (0%)	81	66	107, 181, 263, 360	0
All	All	1713/2040 (83%)	-0.15	23 (1%)	75	59	104, 178, 249, 439	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	TYR	7.6
1	H	13	TYR	7.2
1	C	13	TYR	6.9
1	G	13	TYR	5.1
1	E	13	TYR	4.8
1	H	10	PHE	4.3
1	F	13	TYR	3.3
1	D	13	TYR	3.0
1	B	10	PHE	2.8
1	B	174	PHE	2.8
1	D	114	LEU	2.8
1	B	9	ILE	2.5
1	B	124	LEU	2.3
1	A	104	ALA	2.3
1	C	124	LEU	2.3
1	A	13	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	220	SER	2.2
1	G	10	PHE	2.2
1	A	145	ILE	2.2
1	E	217	GLY	2.1
1	C	103	ILE	2.1
1	C	192	LEU	2.1
1	A	120	VAL	2.1

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.