



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:47 AM GMT

PDB ID : 3G07
Title : Methyltransferase domain of human Bicoid-interacting protein 3 homolog (Drosophila)
Authors : Wu, H.; Dombrowski, L.; Tempel, W.; McCarthy, A.; Loppnau, P.; Bountra, C.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Min, J.; Plotnikov, A.N.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-01-27
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

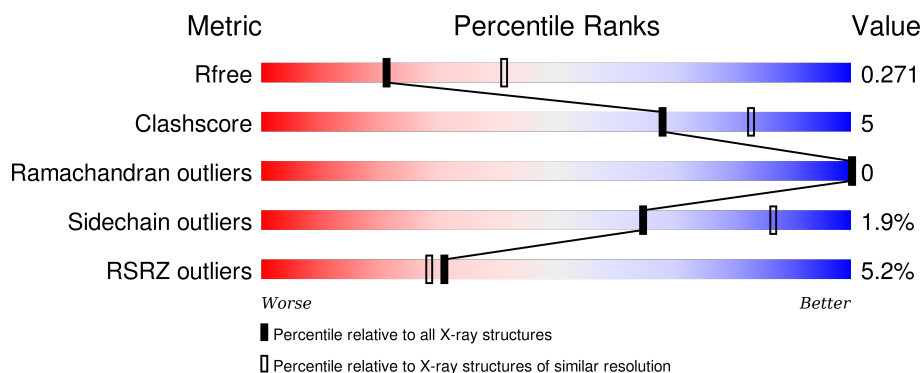
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	292	
1	B	292	
1	C	292	
1	D	292	
1	E	292	

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Mol	Chain	Length	Quality of chain
1	F	292	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '3%', followed by a long green segment labeled '60%', a small yellow segment labeled '6%', and a long grey segment at the end labeled '34%'. The segments are separated by thin white lines.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8567 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.

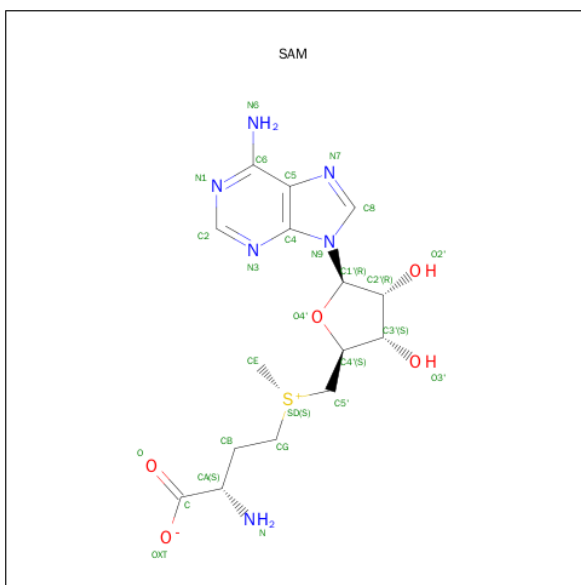
- Molecule 1 is a protein called 7SK snRNA methylphosphate capping enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	Se	0	0	0
			1415	916	239	255	3	2			
1	B	193	Total	C	N	O	S	Se	0	0	0
			1422	919	241	257	3	2			
1	C	190	Total	C	N	O	S	Se	0	0	0
			1386	897	235	249	3	2			
1	D	193	Total	C	N	O	S	Se	0	0	0
			1426	919	242	260	3	2			
1	E	193	Total	C	N	O	S	Se	0	0	0
			1410	911	238	256	3	2			
1	F	193	Total	C	N	O	S	Se	0	0	0
			1346	859	235	247	3	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	GLY	-	EXPRESSION TAG	UNP Q7L2J0
A	399	SER	-	EXPRESSION TAG	UNP Q7L2J0
B	398	GLY	-	EXPRESSION TAG	UNP Q7L2J0
B	399	SER	-	EXPRESSION TAG	UNP Q7L2J0
C	398	GLY	-	EXPRESSION TAG	UNP Q7L2J0
C	399	SER	-	EXPRESSION TAG	UNP Q7L2J0
D	398	GLY	-	EXPRESSION TAG	UNP Q7L2J0
D	399	SER	-	EXPRESSION TAG	UNP Q7L2J0
E	398	GLY	-	EXPRESSION TAG	UNP Q7L2J0
E	399	SER	-	EXPRESSION TAG	UNP Q7L2J0
F	398	GLY	-	EXPRESSION TAG	UNP Q7L2J0
F	399	SER	-	EXPRESSION TAG	UNP Q7L2J0

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



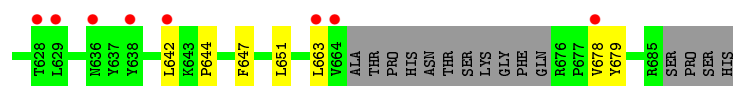
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	B	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	C	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	D	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	E	1	Total 27	C 15	N 6	O 5	S 1	0	0
2	F	1	Total 27	C 15	N 6	O 5	S 1	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

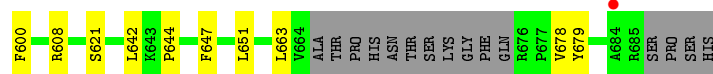
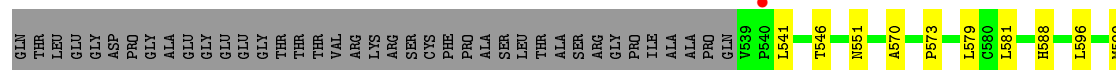
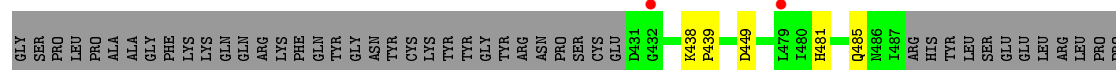
- Chain A:
-
- Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 100. A bar chart at the top indicates the percentage of positions with significant conservation: 4% (red), 55% (green), 11% (yellow), and 34% (grey).
- Conserved residues (bits) are shown below the sequence logo:
- | Position | Residue | Information Content (bits) |
|----------|---------|----------------------------|
| 1 | GLY | 0.15 |
| 2 | SER | 0.15 |
| 3 | PRO | 0.15 |
| 4 | LEU | 0.15 |
| 5 | PRO | 0.15 |
| 6 | ALA | 0.15 |
| 7 | ALA | 0.15 |
| 8 | GLY | 0.15 |
| 9 | PHE | 0.15 |
| 10 | LYS | 0.15 |
| 11 | LYS | 0.15 |
| 12 | GLN | 0.15 |
| 13 | GLN | 0.15 |
| 14 | ARG | 0.15 |
| 15 | LYS | 0.15 |
| 16 | PHE | 0.15 |
| 17 | GLN | 0.15 |
| 18 | TYR | 0.15 |
| 19 | GLY | 0.15 |
| 20 | ASN | 0.15 |
| 21 | ASN | 0.15 |
| 22 | PRO | 0.15 |
| 23 | SER | 0.15 |
| 24 | SER | 0.15 |
| 25 | CYS | 0.15 |
| 26 | GLU | 0.15 |
| 27 | D431 | 0.15 |
| 28 | G432 | 0.15 |
| 29 | R433 | 0.15 |
| 30 | L434 | 0.15 |
| 31 | W441 | 0.15 |
| 32 | L448 | 0.15 |
| 33 | D449 | 0.15 |
| 34 | L450 | 0.15 |
| 35 | G451 | 0.15 |
| 36 | S460 | 0.15 |
| 37 | Y471 | 0.15 |
| 38 | H481 | 0.15 |
| 39 | S482 | 0.15 |
| 40 | Q485 | 0.15 |
| 41 | I486 | 0.15 |
| 42 | I487 | 0.15 |
| 43 | ARG | 0.15 |
| 44 | HIS | 0.15 |
| 45 | TYR | 0.15 |
| 46 | LEU | 0.15 |
| 47 | SER | 0.15 |
| 48 | GLU | 0.15 |
| 49 | GLU | 0.15 |
| 50 | LEU | 0.15 |
| 51 | ARG | 0.15 |
| 52 | LEU | 0.15 |
| 53 | PRO | 0.15 |
| 54 | PRO | 0.15 |
| 55 | GLN | 0.15 |
| 56 | THR | 0.15 |
| 57 | GLU | 0.15 |
| 58 | GLY | 0.15 |
| 59 | ASP | 0.15 |
| 60 | PRO | 0.15 |
| 61 | GLY | 0.15 |
| 62 | ALA | 0.15 |
| 63 | GLU | 0.15 |
| 64 | GLY | 0.15 |
| 65 | GLU | 0.15 |
| 66 | GLY | 0.15 |
| 67 | GLU | 0.15 |
| 68 | GLY | 0.15 |
| 69 | THR | 0.15 |
| 70 | THR | 0.15 |
| 71 | THR | 0.15 |
| 72 | VAL | 0.15 |
| 73 | ARG | 0.15 |
| 74 | LYS | 0.15 |
| 75 | ANG | 0.15 |
| 76 | SER | 0.15 |
| 77 | CYS | 0.15 |
| 78 | PHE | 0.15 |
| 79 | PRO | 0.15 |
| 80 | ALA | 0.15 |
| 81 | SER | 0.15 |
| 82 | LEU | 0.15 |
| 83 | THR | 0.15 |
| 84 | ALA | 0.15 |
| 85 | SER | 0.15 |
| 86 | ANG | 0.15 |
| 87 | GLY | 0.15 |
| 88 | PRO | 0.15 |
| 89 | ILE | 0.15 |
| 90 | ALA | 0.15 |
| 91 | ALA | 0.15 |
| 92 | PRO | 0.15 |
| 93 | GLN | 0.15 |
| 94 | V539 | 0.15 |
| 95 | P540 | 0.15 |
| 96 | L541 | 0.15 |
| 97 | T546 | 0.15 |
| 98 | N551 | 0.15 |
| 99 | Y560 | 0.15 |
| 100 | D563 | 0.15 |
| 101 | A570 | 0.15 |
| 102 | G571 | 0.15 |
| 103 | GLN | 0.15 |
| 104 | R676 | 0.15 |
| 105 | P677 | 0.15 |
| 106 | V678 | 0.15 |
| 107 | V679 | 0.15 |
| 108 | L680 | 0.15 |
| 109 | A684 | 0.15 |
| 110 | R685 | 0.15 |
| 111 | SER | 0.15 |
| 112 | PRO | 0.15 |
| 113 | SER | 0.15 |
| 114 | HIS | 0.15 |

- Chain B:
-
- 3% 58% 9% 34%
- | Amino Acid | Frequency (bits) |
|------------|------------------|
| GLY | 0.00 |
| SER | 0.00 |
| PRO | 0.00 |
| LEU | 0.00 |
| THR | 0.00 |
| ALA | 0.00 |
| ALA | 0.00 |
| GLY | 0.00 |
| PHE | 0.00 |
| LYS | 0.00 |
| GLN | 0.00 |
| GLN | 0.00 |
| ARG | 0.00 |
| LYS | 0.00 |
| PHE | 0.00 |
| GLN | 0.00 |
| THR | 0.00 |
| GLY | 0.00 |
| ASN | 0.00 |
| TYR | 0.00 |
| CYS | 0.00 |
| LYS | 0.00 |
| THR | 0.00 |
| TYR | 0.00 |
| GLY | 0.00 |
| ARG | 0.00 |
| ASN | 0.00 |
| PRO | 0.00 |
| SER | 0.00 |
| CYS | 0.00 |
| GLU | 0.00 |
| D431 | 0.00 |
| G432 | 0.00 |
| K438 | 0.00 |
| P439 | 0.00 |
| L448 | 0.00 |
| D449 | 0.00 |
| L450 | 0.00 |
| V471 | 0.00 |
| H491 | 0.00 |
| S492 | 0.00 |
| Q495 | 0.00 |
| N486 | 0.00 |
| I487 | 0.00 |
| ARG | 0.00 |
| HIS | 0.00 |
| THR | 0.00 |
| LEU | 0.00 |
| SER | 0.00 |
| GLU | 0.00 |
| LEU | 0.00 |
| ASP | 0.00 |
| LEU | 0.00 |
| PRO | 0.00 |
| PRO | 0.00 |
| GLN | 0.00 |
| THR | 0.00 |
| LEU | 0.00 |
| GLU | 0.00 |
| GLY | 0.00 |
| ASP | 0.00 |
| PRO | 0.00 |
| GLY | 0.00 |
| ALA | 0.00 |
| GLU | 0.00 |
| GLY | 0.00 |
| GLU | 0.00 |
| GLY | 0.00 |
| GLY | 0.00 |
| THR | 0.00 |
| THR | 0.00 |
| VAL | 0.00 |
| ARG | 0.00 |
| LYS | 0.00 |
| ARG | 0.00 |
| SER | 0.00 |
| CYS | 0.00 |
| PHE | 0.00 |
| PRO | 0.00 |
| LYS | 0.00 |
| ALA | 0.00 |
| SER | 0.00 |
| LEU | 0.00 |
| THR | 0.00 |
| ALA | 0.00 |
| SER | 0.00 |
| GLY | 0.00 |
| PRO | 0.00 |
| ILE | 0.00 |
| ALA | 0.00 |
| ALA | 0.00 |
| PRO | 0.00 |
| GLN | 0.00 |
| V539 | 0.00 |
| T546 | 0.00 |
| N551 | 0.00 |
| Y560 | 0.00 |
| P573 | 0.00 |
| V578 | 0.00 |
| L579 | 0.00 |
| C580 | 0.00 |
| L581 | 0.00 |
| H588 | 0.00 |
| L596 | 0.00 |
| M599 | 0.00 |
| F600 | 0.00 |
| R608 | 0.00 |
| L615 | 0.00 |
| S621 | 0.00 |
| L642 | 0.00 |
| K643 | 0.00 |
| P644 | 0.00 |
| F647 | 0.00 |
| L651 | 0.00 |
| L663 | 0.00 |
| V664 | 0.00 |
| ALA | 0.00 |
| THR | 0.00 |
| PRO | 0.00 |
| HIS | 0.00 |
| ASN | 0.00 |
| THR | 0.00 |
| SER | 0.00 |
| LYS | 0.00 |
| GLY | 0.00 |
| PHE | 0.00 |
| GLN | 0.00 |
| R676 | 0.00 |
| P677 | 0.00 |
| V678 | 0.00 |
| Y679 | 0.00 |
| R685 | 0.00 |
| SER | 0.00 |
| PRO | 0.00 |
| SER | 0.00 |
| HIS | 0.00 |

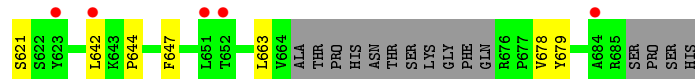
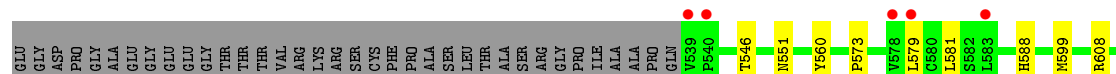
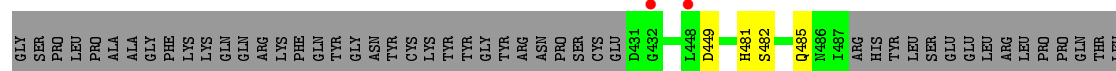
- Chain C:
-
- 5% 59% 7% 35%
- GLY SER PRO LEU PRO ALA ALA GLY PHE GLY LYS GLN GLN ARG THR LYS PHE GLN TYR GLY ASN PRO CYS TYR TYR TYR ASN ARG PRO CYS ASP GLY ARG L434 L448 H481 S482 Q485 N486 I487 ARG HIS TYR LEU SER GLU LEU ARG LEU PRO PRO GLN THR
- LEU GLU GLY ASP PRO GLY ALA GLU GLY GLU GLY THR THR VAL ARG LYS SER CYS PHE PRO ALA SER LEU THR ALA SER ARG PRO ILE ASP ALA PRO GLN V539 T546 N551 L567 P573 C580 L581 H588 L596 M599 F600 R608 L610



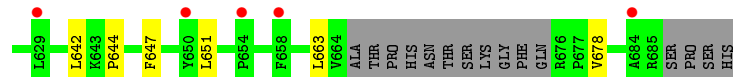
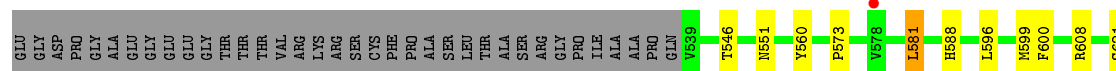
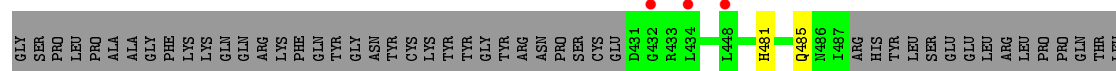
- Molecule 1: 7SK snRNA methylphosphate capping enzyme



- Molecule 1: 7SK snRNA methylphosphate capping enzyme



- Molecule 1: 7SK snRNA methylphosphate capping enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	182.99Å 182.99Å 151.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.70 – 2.65 29.70 – 2.62	Depositor EDS
% Data completeness (in resolution range)	50.0 (29.70-2.65) 99.9 (29.70-2.62)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.265 , 0.282 0.246 , 0.271	Depositor DCC
R_{free} test set	1532 reflections (2.80%)	DCC
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.5	EDS
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 56777 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8567	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	0.30	0/1449	0.46	0/1984
1	B	0.31	0/1456	0.47	0/1992
1	C	0.31	0/1419	0.46	0/1942
1	D	0.33	0/1460	0.47	0/1996
1	E	0.31	0/1445	0.47	0/1979
1	F	0.31	0/1374	0.46	0/1883
All	All	0.31	0/8603	0.47	0/11776

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1415	0	1268	19	0
1	B	1422	0	1281	13	0
1	C	1386	0	1233	10	0
1	D	1426	0	1279	15	0
1	E	1410	0	1239	10	0
1	F	1346	0	1147	11	0
2	A	27	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	22	0	0
2	C	27	0	22	0	0
2	D	27	0	22	0	0
2	E	27	0	22	0	0
2	F	27	0	22	1	0
All	All	8567	0	7579	75	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 5.

All (75) 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:A:434:LEU:HD11	1:A:460:SER:HB3	1.79	0.65
1:A:441:TRP:CZ2	1:A:680:LEU:HD11	2.35	0.61
1:A:570:ALA:HB3	1:D:541:LEU:HD21	1.85	0.57
1:E:481:HIS:O	1:E:485:GLN:HG2	2.04	0.57
1:C:588:HIS:HE1	1:C:642:LEU:O	1.87	0.56
1:F:588:HIS:HE1	1:F:642:LEU:O	1.89	0.56
1:D:481:HIS:O	1:D:485:GLN:HG2	2.07	0.55
1:D:588:HIS:HE1	1:D:642:LEU:O	1.91	0.54
1:A:481:HIS:O	1:A:485:GLN:HG2	2.08	0.54
1:A:588:HIS:HE1	1:A:642:LEU:O	1.91	0.54
1:E:588:HIS:HE1	1:E:642:LEU:O	1.91	0.54
1:C:481:HIS:O	1:C:485:GLN:HG2	2.09	0.53
1:B:588:HIS:HE1	1:B:642:LEU:O	1.91	0.53
1:D:663:LEU:HD13	1:D:679:TYR:CE2	2.44	0.53
1:D:644:PRO:HA	1:D:647:PHE:CE2	2.44	0.53
1:F:644:PRO:HA	1:F:647:PHE:CE2	2.45	0.51
1:B:481:HIS:O	1:B:485:GLN:HG2	2.11	0.51
1:F:481:HIS:O	1:F:485:GLN:HG2	2.11	0.51
1:C:644:PRO:HA	1:C:647:PHE:CE2	2.47	0.50
1:B:663:LEU:HD13	1:B:679:TYR:CE2	2.47	0.50
1:B:644:PRO:HA	1:B:647:PHE:CE2	2.46	0.50
1:F:596:LEU:HD12	1:F:599:MSE:HE2	1.93	0.50
1:E:644:PRO:HA	1:E:647:PHE:CE2	2.47	0.49
1:C:663:LEU:HD12	1:C:678:VAL:O	2.12	0.49
1:A:596:LEU:HD12	1:A:599:MSE:HE2	1.94	0.49
1:C:596:LEU:HD12	1:C:599:MSE:HE2	1.94	0.49
1:D:596:LEU:HD12	1:D:599:MSE:HE2	1.94	0.48
1:A:644:PRO:HA	1:A:647:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:663:LEU:HD12	1:F:678:VAL:O	2.13	0.48
1:D:573:PRO:HB2	1:D:608:ARG:HG2	1.95	0.48
1:C:663:LEU:HD13	1:C:679:TYR:CE2	2.48	0.48
1:A:663:LEU:HD13	1:A:679:TYR:CE2	2.48	0.48
1:A:663:LEU:HD12	1:A:678:VAL:O	2.14	0.48
1:E:663:LEU:HD13	1:E:679:TYR:CE2	2.48	0.48
1:D:600:PHE:CG	1:D:651:LEU:HD21	2.50	0.47
1:E:663:LEU:HD12	1:E:678:VAL:O	2.15	0.47
1:E:546:THR:HA	1:E:551:ASN:HB3	1.97	0.47
1:A:541:LEU:HD21	1:D:570:ALA:HB3	1.96	0.47
1:A:600:PHE:CG	1:A:651:LEU:HD21	2.51	0.46
1:B:596:LEU:HD12	1:B:599:MSE:HE2	1.97	0.46
1:B:663:LEU:HD12	1:B:678:VAL:O	2.16	0.45
1:D:546:THR:HA	1:D:551:ASN:HB3	1.97	0.45
1:F:581:LEU:O	2:F:701:SAM:N	2.50	0.45
1:A:573:PRO:HB2	1:A:608:ARG:HG2	1.98	0.45
1:C:600:PHE:CG	1:C:651:LEU:HD21	2.52	0.45
1:F:573:PRO:HB2	1:F:608:ARG:HG2	1.99	0.45
1:B:573:PRO:HB2	1:B:608:ARG:HG2	1.99	0.45
1:B:546:THR:HA	1:B:551:ASN:HB3	1.99	0.45
1:B:600:PHE:CG	1:B:651:LEU:HD21	2.52	0.44
1:A:546:THR:HA	1:A:551:ASN:HB3	1.99	0.44
1:E:573:PRO:HB2	1:E:608:ARG:HG2	1.99	0.44
1:D:663:LEU:HD12	1:D:678:VAL:O	2.19	0.43
1:F:644:PRO:HA	1:F:647:PHE:CD2	2.53	0.43
1:F:546:THR:HA	1:F:551:ASN:HB3	1.99	0.43
1:B:438:LYS:HA	1:B:439:PRO:HD3	1.89	0.43
1:C:573:PRO:HB2	1:C:608:ARG:HG2	2.00	0.43
1:C:644:PRO:HA	1:C:647:PHE:CD2	2.54	0.43
1:B:644:PRO:HA	1:B:647:PHE:CD2	2.55	0.42
1:F:560:TYR:HD2	1:F:599:MSE:HG3	1.83	0.42
1:E:644:PRO:HA	1:E:647:PHE:CD2	2.55	0.42
1:D:438:LYS:HA	1:D:439:PRO:HD3	1.91	0.42
1:F:600:PHE:CG	1:F:651:LEU:HD21	2.54	0.42
1:A:644:PRO:HA	1:A:647:PHE:CD2	2.55	0.41
1:D:449:ASP:HA	1:D:579:LEU:HB2	2.01	0.41
1:A:584:THR:O	1:A:588:HIS:HB2	2.20	0.41
1:A:451:GLY:O	2:A:701:SAM:HB1	2.19	0.41
1:D:644:PRO:HA	1:D:647:PHE:CD2	2.55	0.41
1:E:560:TYR:HD2	1:E:599:MSE:HG3	1.85	0.41
1:A:449:ASP:HA	1:A:579:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:ASP:HA	1:B:579:LEU:HB2	2.02	0.41
1:C:546:THR:HA	1:C:551:ASN:HB3	2.03	0.41
1:E:449:ASP:HA	1:E:579:LEU:HB2	2.03	0.41
1:B:560:TYR:HD2	1:B:599:MSE:HG3	1.86	0.40
1:A:571:GLN:HB2	1:D:541:LEU:CD1	2.52	0.40
1:A:560:TYR:HD2	1:A:599:MSE:HG3	1.86	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	187/292 (64%)	177 (95%)	10 (5%)	0	100	100
1	B	187/292 (64%)	177 (95%)	10 (5%)	0	100	100
1	C	184/292 (63%)	175 (95%)	9 (5%)	0	100	100
1	D	187/292 (64%)	177 (95%)	10 (5%)	0	100	100
1	E	187/292 (64%)	178 (95%)	9 (5%)	0	100	100
1	F	187/292 (64%)	177 (95%)	10 (5%)	0	100	100
All	All	1119/1752 (64%)	1061 (95%)	58 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	132/253 (52%)	129 (98%)	3 (2%)	58	83
1	B	134/253 (53%)	131 (98%)	3 (2%)	60	84
1	C	127/253 (50%)	125 (98%)	2 (2%)	70	89
1	D	135/253 (53%)	133 (98%)	2 (2%)	72	90
1	E	128/253 (51%)	125 (98%)	3 (2%)	58	83
1	F	114/253 (45%)	112 (98%)	2 (2%)	66	88
All	All	770/1518 (51%)	755 (98%)	15 (2%)	65	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	SER
1	A	581	LEU
1	A	621	SER
1	B	482	SER
1	B	581	LEU
1	B	621	SER
1	C	482	SER
1	C	581	LEU
1	D	581	LEU
1	D	621	SER
1	E	482	SER
1	E	581	LEU
1	E	621	SER
1	F	581	LEU
1	F	621	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAM	A	701	-	21,29,29	1.06	2 (9%)	17,42,42	2.66	1 (5%)
2	SAM	B	701	-	21,29,29	1.02	2 (9%)	17,42,42	3.05	2 (11%)
2	SAM	C	701	-	21,29,29	1.06	2 (9%)	17,42,42	2.98	3 (17%)
2	SAM	D	701	-	21,29,29	1.08	2 (9%)	17,42,42	2.90	1 (5%)
2	SAM	E	701	-	21,29,29	1.08	2 (9%)	17,42,42	2.78	1 (5%)
2	SAM	F	701	-	21,29,29	1.04	2 (9%)	17,42,42	2.84	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAM	A	701	-	-	0/8/33/33	0/3/3/3
2	SAM	B	701	-	-	0/8/33/33	0/3/3/3
2	SAM	C	701	-	-	0/8/33/33	0/3/3/3
2	SAM	D	701	-	-	0/8/33/33	0/3/3/3
2	SAM	E	701	-	-	0/8/33/33	0/3/3/3
2	SAM	F	701	-	-	0/8/33/33	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	SAM	C2-N1	2.16	1.38	1.33
2	B	701	SAM	C2-N1	2.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	SAM	C2-N1	2.25	1.38	1.33
2	F	701	SAM	C2-N1	2.37	1.38	1.33
2	C	701	SAM	C2-N1	2.38	1.38	1.33
2	A	701	SAM	C2-N1	2.43	1.38	1.33
2	B	701	SAM	C2-N3	2.81	1.37	1.32
2	F	701	SAM	C2-N3	3.30	1.38	1.32
2	D	701	SAM	C2-N3	3.38	1.38	1.32
2	A	701	SAM	C2-N3	3.39	1.38	1.32
2	C	701	SAM	C2-N3	3.43	1.38	1.32
2	E	701	SAM	C2-N3	3.63	1.38	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	SAM	N3-C2-N1	-11.93	119.76	128.89
2	C	701	SAM	N3-C2-N1	-11.58	120.03	128.89
2	D	701	SAM	N3-C2-N1	-11.39	120.17	128.89
2	F	701	SAM	N3-C2-N1	-11.01	120.46	128.89
2	E	701	SAM	N3-C2-N1	-10.93	120.53	128.89
2	A	701	SAM	N3-C2-N1	-10.56	120.81	128.89
2	C	701	SAM	C1'-N9-C4	-2.40	123.32	126.94
2	F	701	SAM	C1'-N9-C4	-2.36	123.38	126.94
2	B	701	SAM	C1'-N9-C4	-2.31	123.46	126.94
2	F	701	SAM	C4-C5-N7	-2.29	107.37	109.48
2	C	701	SAM	C4-C5-N7	-2.01	107.63	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	SAM	1	0
2	F	701	SAM	1	0

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	191/292 (65%)	0.31	11 (5%) 26 24	54, 85, 121, 136	0
1	B	191/292 (65%)	0.28	9 (4%) 35 33	48, 81, 118, 133	0
1	C	188/292 (64%)	0.34	14 (7%) 17 14	55, 87, 125, 138	0
1	D	191/292 (65%)	0.07	4 (2%) 67 66	52, 84, 121, 134	0
1	E	191/292 (65%)	0.10	12 (6%) 23 21	56, 84, 121, 137	0
1	F	191/292 (65%)	0.27	9 (4%) 35 33	58, 92, 128, 139	0
All	All	1143/1752 (65%)	0.23	59 (5%) 31 28	48, 85, 123, 139	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	629	LEU	5.7
1	C	628	THR	5.4
1	C	642	LEU	5.0
1	A	432	GLY	4.4
1	A	684	ALA	4.3
1	B	580	CYS	4.2
1	D	432	GLY	3.9
1	C	486	ASN	3.8
1	C	580	CYS	3.5
1	F	684	ALA	3.4
1	E	539	VAL	3.3
1	B	450	LEU	3.3
1	C	567	LEU	3.1
1	E	579	LEU	3.1
1	A	580	CYS	3.0
1	D	540	PRO	2.9
1	C	638	TYR	2.9
1	C	619	PRO	2.9
1	F	650	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	658	PHE	2.8
1	A	615	LEU	2.8
1	D	684	ALA	2.8
1	F	654	PRO	2.8
1	B	448	LEU	2.7
1	A	579	LEU	2.7
1	C	636	ASN	2.6
1	E	578	VAL	2.6
1	B	579	LEU	2.6
1	E	583	LEU	2.5
1	E	432	GLY	2.5
1	B	578	VAL	2.5
1	F	434	LEU	2.5
1	A	634	TYR	2.5
1	C	678	VAL	2.5
1	A	563	ASP	2.4
1	F	432	GLY	2.4
1	A	471	VAL	2.4
1	C	539	VAL	2.4
1	A	448	LEU	2.3
1	B	432	GLY	2.3
1	F	448	LEU	2.2
1	E	540	PRO	2.2
1	B	471	VAL	2.2
1	C	448	LEU	2.2
1	E	623	TYR	2.2
1	C	629	LEU	2.2
1	E	642	LEU	2.2
1	A	659	SER	2.1
1	B	486	ASN	2.1
1	A	431	ASP	2.1
1	E	651	LEU	2.1
1	B	615	LEU	2.1
1	C	664	VAL	2.1
1	E	448	LEU	2.1
1	C	663	LEU	2.1
1	E	652	THR	2.0
1	D	479	LEU	2.0
1	E	684	ALA	2.0
1	F	578	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SAM	E	701	27/27	0.95	0.20	-0.18	61,70,89,159	0
2	SAM	D	701	27/27	0.96	0.17	-0.36	55,69,88,158	0
2	SAM	B	701	27/27	0.97	0.18	-0.37	48,62,93,154	0
2	SAM	F	701	27/27	0.95	0.15	-0.57	67,84,116,128	0
2	SAM	A	701	27/27	0.95	0.17	-0.68	58,70,95,168	0
2	SAM	C	701	27/27	0.97	0.14	-1.12	60,72,118,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.