



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 10:55 PM UTC

PDB ID : 6BI7 / pdb_00006bi7
Title : Crystal structure of Rev7-WT/Rev3 as a monomer under high-salt conditions
Authors : Rizzo, A.A.; Korzhnev, D.M.; Hao, B.; Li, Y.
Deposited on : 2017-11-01
Resolution : 2.80 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:

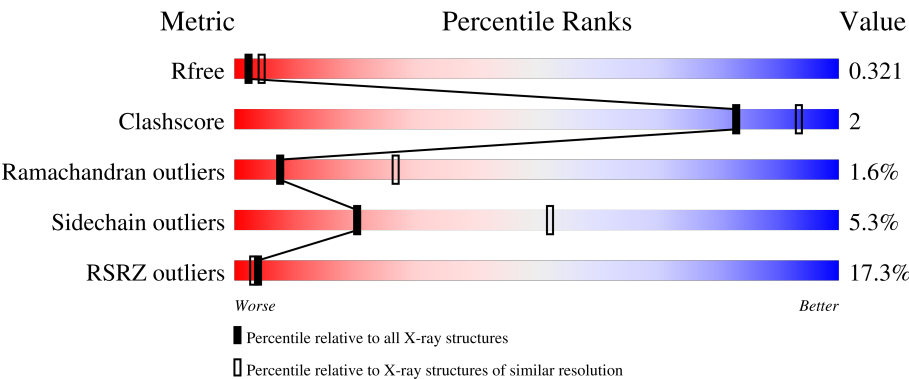
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	227	9% 68% 11% •• 18%
1	C	227	8% 69% 9% • 20%
1	E	227	16% 66% 8% •• 23%
1	G	227	24% 62% 6% 32%
2	B	28	79% • 18%

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Mol	Chain	Length	Quality of chain
2	D	28	4% 89% 7%
2	F	28	11% 71% 25%
2	H	28	7% 75% 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6445 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 Mitotic spindle assembly checkpoint protein MAD2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1522	989	254	269	10			
1	C	182	Total	C	N	O	S	0	0	0
			1498	971	252	265	10			
1	E	174	Total	C	N	O	S	0	0	0
			1420	926	231	254	9			
1	G	154	Total	C	N	O	S	0	0	0
			1257	823	204	222	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q9UI95
A	-14	GLY	-	expression tag	UNP Q9UI95
A	-13	SER	-	expression tag	UNP Q9UI95
A	-12	SER	-	expression tag	UNP Q9UI95
A	-11	HIS	-	expression tag	UNP Q9UI95
A	-10	HIS	-	expression tag	UNP Q9UI95
A	-9	HIS	-	expression tag	UNP Q9UI95
A	-8	HIS	-	expression tag	UNP Q9UI95
A	-7	HIS	-	expression tag	UNP Q9UI95
A	-6	HIS	-	expression tag	UNP Q9UI95
A	-5	SER	-	expression tag	UNP Q9UI95
A	-4	GLN	-	expression tag	UNP Q9UI95
A	-3	ASP	-	expression tag	UNP Q9UI95
A	-2	PRO	-	expression tag	UNP Q9UI95
A	-1	ASN	-	expression tag	UNP Q9UI95
A	0	SER	-	expression tag	UNP Q9UI95
C	-15	MET	-	initiating methionine	UNP Q9UI95
C	-14	GLY	-	expression tag	UNP Q9UI95
C	-13	SER	-	expression tag	UNP Q9UI95
C	-12	SER	-	expression tag	UNP Q9UI95
C	-11	HIS	-	expression tag	UNP Q9UI95

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP Q9UI95
C	-9	HIS	-	expression tag	UNP Q9UI95
C	-8	HIS	-	expression tag	UNP Q9UI95
C	-7	HIS	-	expression tag	UNP Q9UI95
C	-6	HIS	-	expression tag	UNP Q9UI95
C	-5	SER	-	expression tag	UNP Q9UI95
C	-4	GLN	-	expression tag	UNP Q9UI95
C	-3	ASP	-	expression tag	UNP Q9UI95
C	-2	PRO	-	expression tag	UNP Q9UI95
C	-1	ASN	-	expression tag	UNP Q9UI95
C	0	SER	-	expression tag	UNP Q9UI95
E	-15	MET	-	initiating methionine	UNP Q9UI95
E	-14	GLY	-	expression tag	UNP Q9UI95
E	-13	SER	-	expression tag	UNP Q9UI95
E	-12	SER	-	expression tag	UNP Q9UI95
E	-11	HIS	-	expression tag	UNP Q9UI95
E	-10	HIS	-	expression tag	UNP Q9UI95
E	-9	HIS	-	expression tag	UNP Q9UI95
E	-8	HIS	-	expression tag	UNP Q9UI95
E	-7	HIS	-	expression tag	UNP Q9UI95
E	-6	HIS	-	expression tag	UNP Q9UI95
E	-5	SER	-	expression tag	UNP Q9UI95
E	-4	GLN	-	expression tag	UNP Q9UI95
E	-3	ASP	-	expression tag	UNP Q9UI95
E	-2	PRO	-	expression tag	UNP Q9UI95
E	-1	ASN	-	expression tag	UNP Q9UI95
E	0	SER	-	expression tag	UNP Q9UI95
G	-15	MET	-	initiating methionine	UNP Q9UI95
G	-14	GLY	-	expression tag	UNP Q9UI95
G	-13	SER	-	expression tag	UNP Q9UI95
G	-12	SER	-	expression tag	UNP Q9UI95
G	-11	HIS	-	expression tag	UNP Q9UI95
G	-10	HIS	-	expression tag	UNP Q9UI95
G	-9	HIS	-	expression tag	UNP Q9UI95
G	-8	HIS	-	expression tag	UNP Q9UI95
G	-7	HIS	-	expression tag	UNP Q9UI95
G	-6	HIS	-	expression tag	UNP Q9UI95
G	-5	SER	-	expression tag	UNP Q9UI95
G	-4	GLN	-	expression tag	UNP Q9UI95
G	-3	ASP	-	expression tag	UNP Q9UI95
G	-2	PRO	-	expression tag	UNP Q9UI95
G	-1	ASN	-	expression tag	UNP Q9UI95

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP Q9UI95

- Molecule 2 is a protein called DNA polymerase zeta catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	S	0	1	0
			188	123	34	28	3			
2	D	26	Total	C	N	O	S	0	0	0
			208	134	37	34	3			
2	F	21	Total	C	N	O	S	0	0	0
			165	107	30	25	3			
2	H	22	Total	C	N	O	S	0	0	0
			174	112	31	28	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1987	MET	-	initiating methionine	UNP O60673
D	1987	MET	-	initiating methionine	UNP O60673
F	1987	MET	-	initiating methionine	UNP O60673
H	1987	MET	-	initiating methionine	UNP O60673

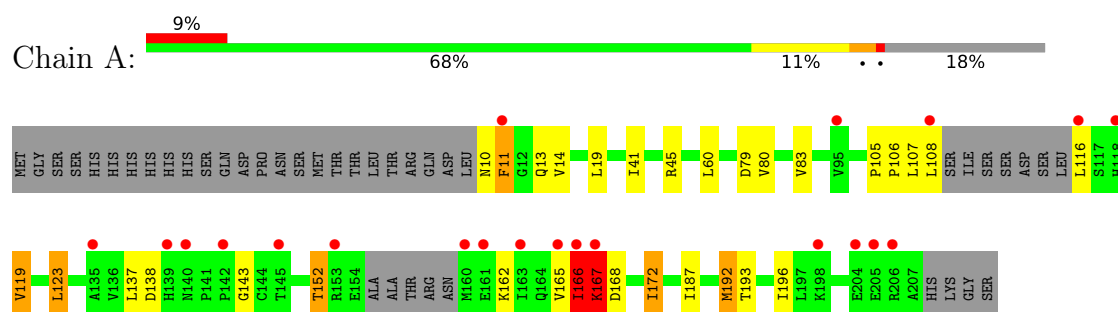
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	C	2	Total	O	0	0
			2	2		
3	E	3	Total	O	0	0
			3	3		
3	G	3	Total	O	0	0
			3	3		

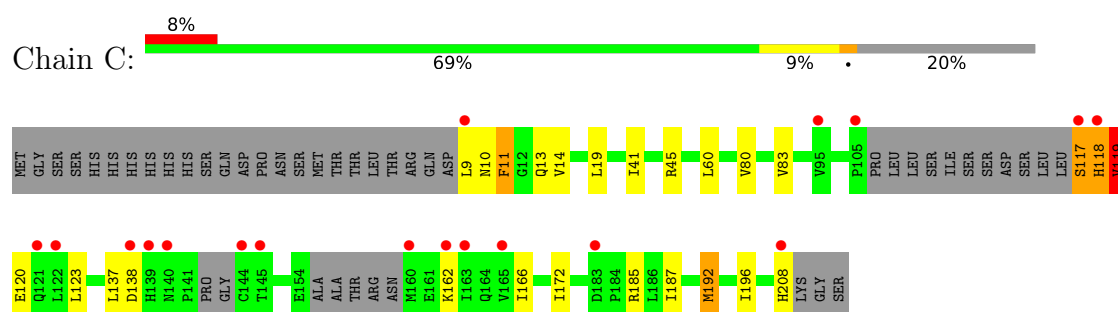
3 Residue-property plots [i](#)

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.

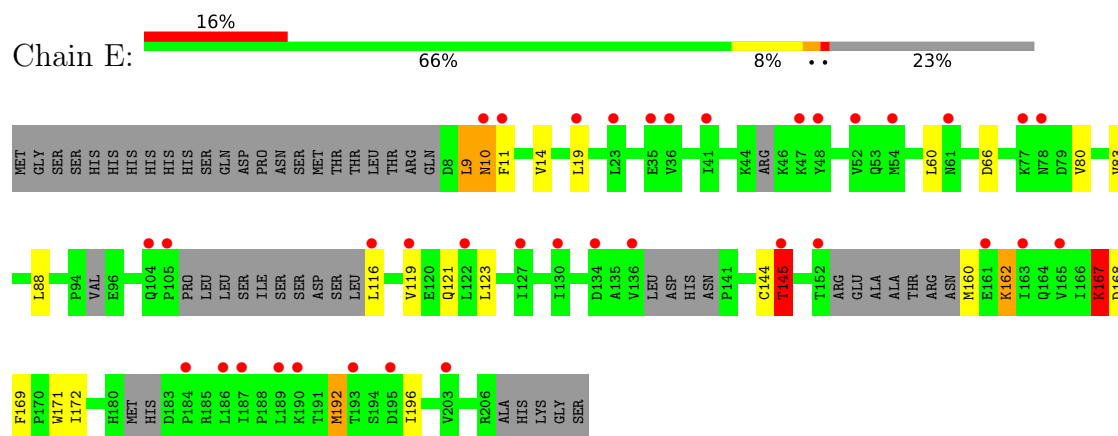
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B



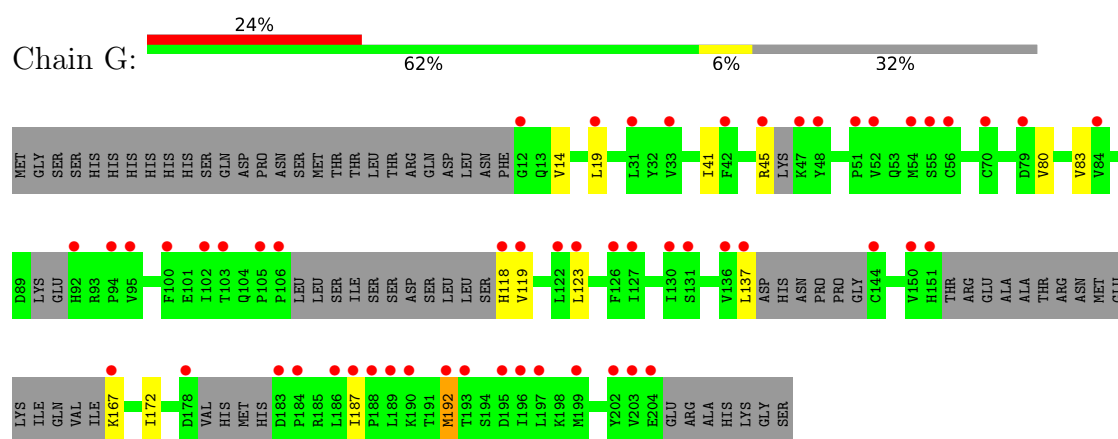
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B



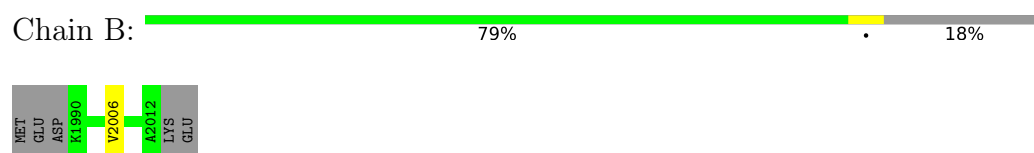
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B



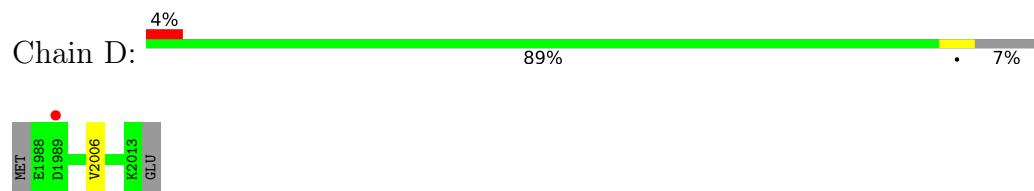
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2B



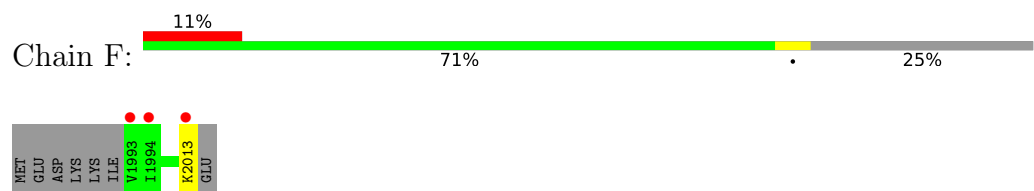
- Molecule 2: DNA polymerase zeta catalytic subunit



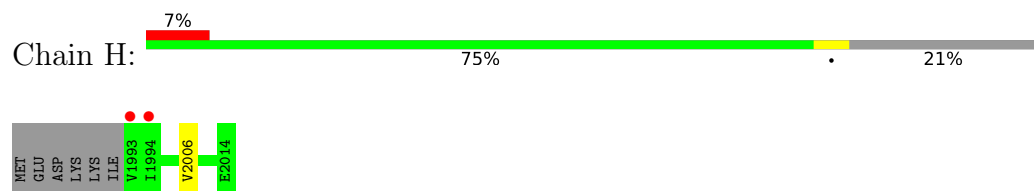
- Molecule 2: DNA polymerase zeta catalytic subunit



- Molecule 2: DNA polymerase zeta catalytic subunit



- Molecule 2: DNA polymerase zeta catalytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.70Å 89.70Å 284.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	284.84 – 2.80 94.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (284.84-2.80) 99.8 (94.95-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.275 , 0.321 0.275 , 0.321	Depositor DCC
R_{free} test set	1715 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6445	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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	0.81	1/1555 (0.1%)	1.03	6/2111 (0.3%)
1	C	0.80	1/1529 (0.1%)	0.98	6/2072 (0.3%)
1	E	0.73	1/1446 (0.1%)	0.98	4/1956 (0.2%)
1	G	0.62	0/1280	0.90	1/1735 (0.1%)
2	B	0.69	0/194	0.95	0/261
2	D	0.67	0/211	0.92	0/283
2	F	0.65	0/168	0.92	0/227
2	H	0.63	0/177	0.83	0/239
All	All	0.74	3/6560 (0.0%)	0.97	17/8884 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	PRO	CA-C	6.80	1.56	1.52
1	E	145	THR	N-CA	5.89	1.53	1.46
1	C	117	SER	CA-CB	5.77	1.65	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	GLN	N-CA-C	-7.68	102.50	111.03
1	E	145	THR	N-CA-C	7.53	126.84	110.80
1	G	119	VAL	N-CA-C	-7.08	103.95	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ILE	N-CA-C	-6.86	95.07	109.34
1	A	119	VAL	N-CA-C	-6.44	104.57	110.82
1	A	11	PHE	N-CA-C	-6.43	100.95	110.46
1	C	13	GLN	N-CA-C	-6.23	104.11	111.03
1	A	60	LEU	N-CA-C	-6.21	104.44	111.14
1	C	119	VAL	N-CA-CB	5.99	121.69	111.50
1	C	117	SER	CB-CA-C	5.81	121.13	110.10
1	C	60	LEU	N-CA-C	-5.73	104.41	111.40
1	E	119	VAL	N-CA-C	-5.63	105.36	110.82
1	C	11	PHE	N-CA-C	-5.44	102.41	110.46
1	A	105	PRO	CB-CA-C	5.39	116.24	111.17
1	E	162	LYS	CA-CB-CG	5.29	124.68	114.10
1	E	60	LEU	N-CA-C	-5.14	105.59	111.14
1	C	166	ILE	N-CA-C	5.04	115.27	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	118	HIS	Peptide
1	E	9	LEU	Peptide

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	1522	0	1561	14	0
1	C	1498	0	1528	7	0
1	E	1420	0	1454	8	0
1	G	1257	0	1289	4	0
2	B	188	0	212	1	0
2	D	208	0	227	1	0
2	F	165	0	180	0	0
2	H	174	0	186	1	0
3	A	5	0	0	2	0
3	C	2	0	0	0	0
3	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	3	0	0	0	0
All	All	6445	0	6637	31	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 2.

All (31) 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:166:ILE:O	1:A:168:ASP:N	2.19	0.74
1:A:193:THR:OG1	1:C:185:ARG:NH2	2.24	0.70
1:E:167:LYS:O	1:E:169:PHE:N	2.34	0.61
1:A:165:VAL:C	1:A:166:ILE:O	2.43	0.58
1:A:166:ILE:HG22	1:A:167:LYS:H	1.70	0.57
1:A:137:LEU:HD23	1:A:187:ILE:HD13	1.88	0.56
1:G:41:ILE:HG21	2:H:2006:VAL:CG1	2.36	0.55
1:A:123:LEU:CD1	1:A:192:MET:HE1	2.37	0.55
1:C:137:LEU:HD23	1:C:187:ILE:HD13	1.90	0.54
1:G:137:LEU:HD23	1:G:187:ILE:HD13	1.90	0.54
1:C:41:ILE:HG21	2:D:2006:VAL:CG1	2.40	0.51
1:E:88:LEU:O	1:E:144:CYS:O	2.27	0.51
1:E:11:PHE:CZ	1:E:196:ILE:HG22	2.48	0.48
1:C:118:HIS:HA	1:C:120:GLU:H	1.79	0.47
1:C:11:PHE:CZ	1:C:196:ILE:HG22	2.50	0.46
1:A:108:LEU:HD11	1:E:121:GLN:HE22	1.80	0.46
1:A:11:PHE:CZ	1:A:196:ILE:HG22	2.51	0.45
1:E:66:ASP:OD2	1:E:167:LYS:HE3	2.16	0.45
1:A:41:ILE:HG21	2:B:2006:VAL:CG1	2.47	0.44
1:A:172:ILE:HD13	3:A:304:HOH:O	2.17	0.44
1:A:79:ASP:O	1:A:152:THR:HG23	2.19	0.42
1:A:80:VAL:HG11	1:A:83:VAL:HG23	2.02	0.42
1:C:123:LEU:HD23	1:C:192:MET:HE1	2.01	0.42
1:A:119:VAL:HG12	1:A:123:LEU:HD22	2.00	0.42
1:A:172:ILE:CD1	3:A:304:HOH:O	2.68	0.42
1:C:80:VAL:HG11	1:C:83:VAL:HG23	2.02	0.42
1:E:80:VAL:HG11	1:E:83:VAL:HG23	2.02	0.41
1:G:123:LEU:HD23	1:G:192:MET:HE1	2.02	0.41
1:E:160:MET:HE1	1:E:171:TRP:CD1	2.55	0.41
1:G:80:VAL:HG11	1:G:83:VAL:HG23	2.03	0.40
1:E:123:LEU:HD23	1:E:192:MET:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/227 (79%)	169 (94%)	6 (3%)	5 (3%)	4	14
1	C	174/227 (77%)	166 (95%)	6 (3%)	2 (1%)	11	36
1	E	160/227 (70%)	149 (93%)	6 (4%)	5 (3%)	3	12
1	G	140/227 (62%)	135 (96%)	5 (4%)	0	100	100
2	B	22/28 (79%)	22 (100%)	0	0	100	100
2	D	24/28 (86%)	23 (96%)	1 (4%)	0	100	100
2	F	19/28 (68%)	18 (95%)	1 (5%)	0	100	100
2	H	20/28 (71%)	18 (90%)	2 (10%)	0	100	100
All	All	739/1020 (72%)	700 (95%)	27 (4%)	12 (2%)	7	27

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ILE
1	A	167	LYS
1	E	10	ASN
1	E	145	THR
1	A	162	LYS
1	C	162	LYS
1	E	162	LYS
1	E	167	LYS
1	C	119	VAL
1	E	168	ASP
1	A	106	PRO
1	A	143	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	177/214 (83%)	165 (93%)	12 (7%)	14	42
1	C	174/214 (81%)	163 (94%)	11 (6%)	16	45
1	E	166/214 (78%)	157 (95%)	9 (5%)	20	51
1	G	147/214 (69%)	140 (95%)	7 (5%)	23	56
2	B	22/26 (85%)	22 (100%)	0	100	100
2	D	24/26 (92%)	24 (100%)	0	100	100
2	F	19/26 (73%)	18 (95%)	1 (5%)	20	52
2	H	20/26 (77%)	20 (100%)	0	100	100
All	All	749/960 (78%)	709 (95%)	40 (5%)	20	52

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	14	VAL
1	A	19	LEU
1	A	45	ARG
1	A	107	LEU
1	A	116	LEU
1	A	123	LEU
1	A	138	ASP
1	A	152	THR
1	A	167	LYS
1	A	172	ILE
1	A	192	MET
1	C	9	LEU
1	C	10	ASN
1	C	14	VAL
1	C	19	LEU
1	C	45	ARG
1	C	117	SER
1	C	119	VAL

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Mol	Chain	Res	Type
1	C	138	ASP
1	C	172	ILE
1	C	192	MET
1	C	208	HIS
1	E	9	LEU
1	E	10	ASN
1	E	14	VAL
1	E	19	LEU
1	E	116	LEU
1	E	145	THR
1	E	167	LYS
1	E	172	ILE
1	E	192	MET
2	F	2013	LYS
1	G	14	VAL
1	G	19	LEU
1	G	45	ARG
1	G	118	HIS
1	G	167	LYS
1	G	172	ILE
1	G	192	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	78	ASN
1	A	140	ASN
2	B	2011	GLN
1	C	43	GLN
1	C	140	ASN
2	D	2011	GLN
1	E	57	HIS
1	E	78	ASN
1	E	121	GLN
2	F	2007	GLN
2	F	2011	GLN
2	H	2007	GLN
2	H	2011	GLN

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

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	186/227 (81%)	0.83	21 (11%)	10 7	44, 71, 130, 161	0
1	C	182/227 (80%)	0.67	18 (9%)	13 9	40, 68, 126, 152	0
1	E	174/227 (76%)	1.27	36 (20%)	2 2	63, 112, 161, 172	0
1	G	154/227 (67%)	1.69	55 (35%)	1 0	61, 114, 169, 219	0
2	B	23/28 (82%)	0.29	0	100 100	40, 71, 100, 123	1 (4%)
2	D	26/28 (92%)	0.37	1 (3%)	44 35	57, 73, 115, 133	0
2	F	21/28 (75%)	0.84	3 (14%)	6 5	75, 91, 112, 125	0
2	H	22/28 (78%)	0.58	2 (9%)	15 11	72, 92, 116, 143	0
All	All	788/1020 (77%)	1.02	136 (17%)	4 3	40, 89, 152, 219	1 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	102	ILE	4.9
1	G	187	ILE	4.4
1	C	9	LEU	4.4
1	C	105	PRO	4.4
1	C	122	LEU	4.4
1	E	11	PHE	4.3
1	G	94	PRO	4.3
1	G	95	VAL	4.1
1	E	122	LEU	4.1
1	G	56	CYS	4.1
1	C	140	ASN	4.0
1	G	189	LEU	4.0
1	G	119	VAL	4.0
1	G	196	ILE	3.9
1	E	105	PRO	3.9
1	G	197	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	192	MET	3.8
1	G	193	THR	3.8
1	A	167	LYS	3.7
1	A	153	ARG	3.7
1	C	138	ASP	3.7
1	G	48	TYR	3.7
1	G	52	VAL	3.7
1	G	127	ILE	3.7
1	G	186	LEU	3.6
1	G	33	VAL	3.6
1	E	48	TYR	3.5
1	G	199	MET	3.5
1	G	190	LYS	3.5
1	A	160	MET	3.5
1	G	204	GLU	3.5
1	G	178	ASP	3.5
1	E	145	THR	3.5
1	A	11	PHE	3.4
1	E	189	LEU	3.4
1	E	47	LYS	3.4
1	G	118	HIS	3.3
1	G	137	LEU	3.3
1	G	42	PHE	3.3
1	G	45	ARG	3.3
1	E	54	MET	3.2
1	A	166	ILE	3.2
1	G	105	PRO	3.2
1	E	136	VAL	3.1
1	G	79	ASP	3.1
1	C	145	THR	3.1
1	A	145	THR	3.1
1	E	152	THR	3.1
1	G	203	VAL	3.0
1	G	195	ASP	3.0
1	E	119	VAL	3.0
1	C	183	ASP	3.0
1	G	84	VAL	3.0
1	C	118	HIS	2.9
1	A	140	ASN	2.9
1	E	116	LEU	2.9
1	G	184	PRO	2.9
1	E	23	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	167	LYS	2.8
1	G	70	CYS	2.8
1	A	198	LYS	2.8
1	A	139	HIS	2.8
1	G	12	GLY	2.8
2	H	1993	VAL	2.8
1	A	204	GLU	2.8
1	G	150	VAL	2.8
1	G	103	THR	2.7
1	C	117	SER	2.7
1	G	188	PRO	2.7
1	E	104	GLN	2.7
1	C	95	VAL	2.7
2	F	1993	VAL	2.7
1	E	77	LYS	2.6
1	A	95	VAL	2.6
1	E	186	LEU	2.6
1	E	41	ILE	2.6
1	A	108	LEU	2.6
1	G	106	PRO	2.6
1	A	135	ALA	2.5
1	A	206	ARG	2.5
1	A	142	PRO	2.5
1	G	123	LEU	2.5
1	G	126	PHE	2.5
1	G	55	SER	2.5
1	E	78	ASN	2.5
1	E	184	PRO	2.4
1	G	202	TYR	2.4
1	E	193	THR	2.4
1	G	92	HIS	2.4
1	E	10	ASN	2.4
1	G	54	MET	2.4
1	E	130	ILE	2.4
1	A	165	VAL	2.4
1	E	52	VAL	2.4
1	C	160	MET	2.4
1	G	151	HIS	2.4
1	G	122	LEU	2.4
1	E	165	VAL	2.4
2	F	2013	LYS	2.3
1	G	100	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	136	VAL	2.3
1	E	19	LEU	2.3
1	G	31	LEU	2.3
2	D	1989	ASP	2.3
1	E	190	LYS	2.3
1	A	163	ILE	2.3
1	E	127	ILE	2.3
1	G	130	ILE	2.3
1	E	161	GLU	2.2
1	G	47	LYS	2.2
1	A	118	HIS	2.2
1	C	163	ILE	2.2
2	H	1994	ILE	2.2
1	C	144	CYS	2.2
1	A	161	GLU	2.2
1	G	183	ASP	2.2
1	C	208	HIS	2.2
1	E	134	ASP	2.2
1	C	162	LYS	2.2
1	E	187	ILE	2.1
2	F	1994	ILE	2.1
1	E	35	GLU	2.1
1	G	144	CYS	2.1
1	E	36	VAL	2.1
1	G	51	PRO	2.1
1	C	139	HIS	2.1
1	E	203	VAL	2.1
1	E	61	ASN	2.1
1	E	195	ASP	2.1
1	A	116	LEU	2.0
1	E	163	ILE	2.0
1	A	205	GLU	2.0
1	C	121	GLN	2.0
1	G	131	SER	2.0
1	G	19	LEU	2.0
1	C	165	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.