



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:36 PM UTC

PDB ID : 5UI8 / pdb_00005ui8
Title : structure of sigmaN-holoenzyme
Authors : Darst, S.A.; Campbell, E.A.
Deposited on : 2017-01-13
Resolution : 3.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

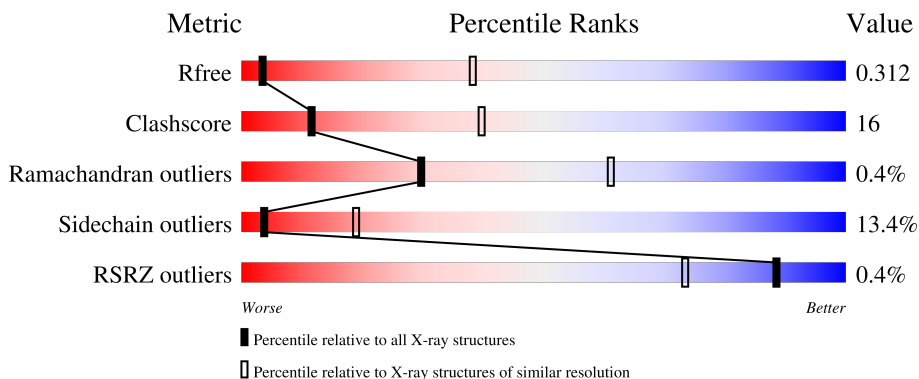
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.76 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.



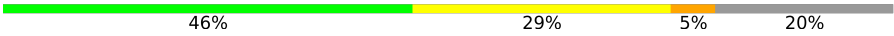
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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 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	G	329	 59% 30% 5% 6%
1	H	329	 41% 21% 1% 35%
2	I	1342	 54% 32% 5% 9%
3	J	1407	 58% 32% 5% 5%
4	K	91	 52% 29% 7% 13%

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Mol	Chain	Length	Quality of chain
5	M	477	 46% 29% 5% 20%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 27004 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	309	Total	C	N	O	S	0	0	0
			2337	1463	408	459	7			
1	H	215	Total	C	N	O	S	0	0	0
			1619	1013	279	321	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	1217	Total	C	N	O	S	0	0	0
			9382	5883	1632	1827	40			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	516	VAL	ASP	conflict	UNP B7MIX3

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	J	1336	Total	C	N	O	S	0	0	0
			10148	6364	1812	1923	49			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	K	79	Total	C	N	O	S	0	0	0
			620	377	118	124	1			

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	M	380	2895	1825	499	561	10	0	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	J	1	1	1	0	0

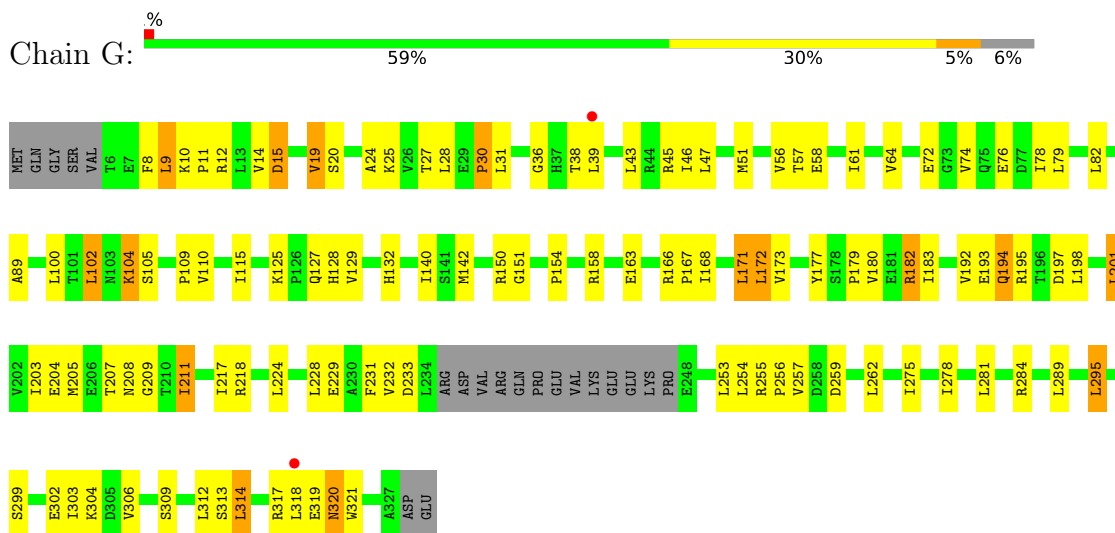
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	J	2	2	2	0	0

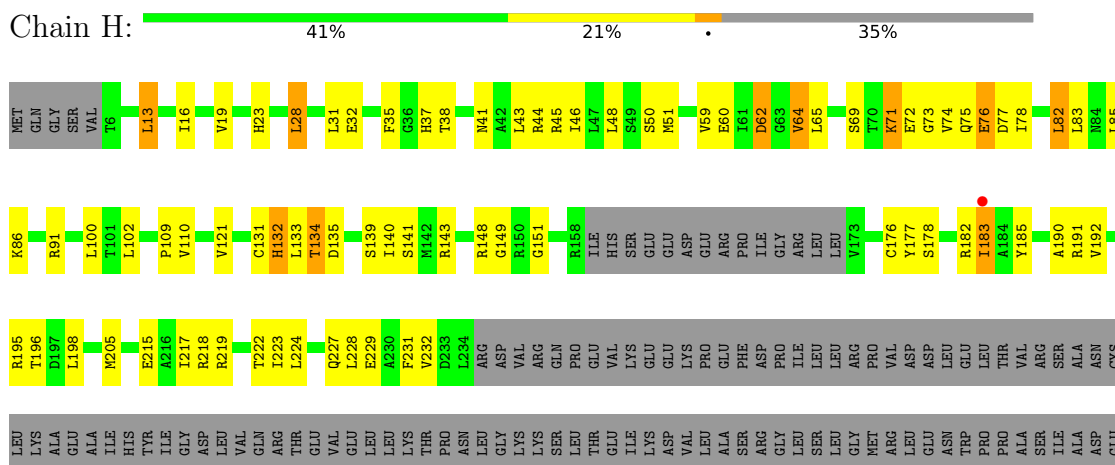
3 Residue-property plots [i](#)

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: DNA-directed RNA polymerase subunit alpha



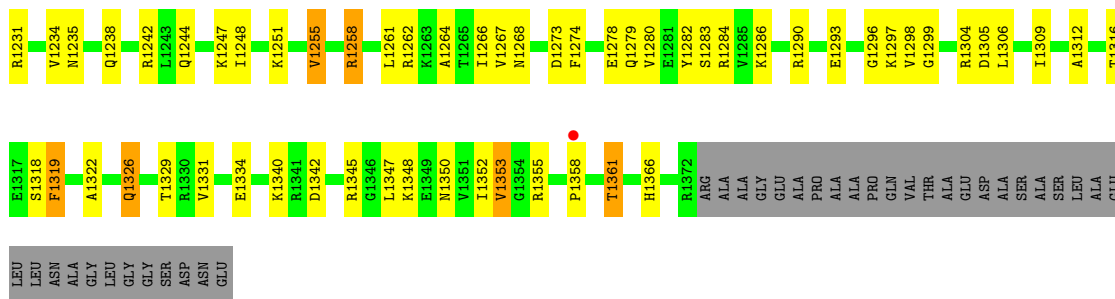
- Molecule 1: DNA-directed RNA polymerase subunit alpha



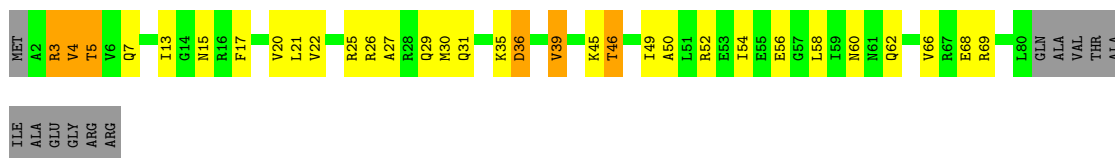
- Molecule 2: DNA-directed RNA polymerase subunit beta



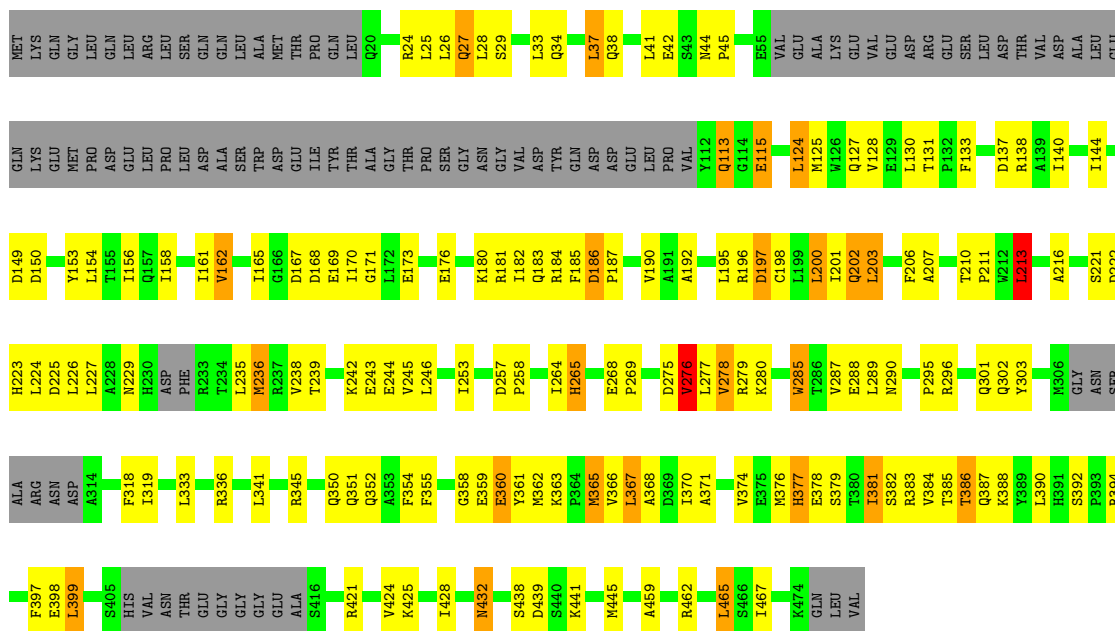
Y1229	R1156	V1075	R976	G885	R801	M685	T689	Q490	L76	S166	ASN	LYS	MET
M1230	Q1157	I1076	L979	K866	M805	Q886	P690	D491	F80	S167	LYS	VAL	V2
M1231	K1158	I1079	V980	R887	P806	R657	V694	M492	F80	S167	LEU	ALA	Y3
L1233	D1160	M1080	L1161	P889	W807	I493	V594	I493	Q83	V170	GLU	ALA	Y4
V1239	L1161	P1081	V884	L895	N808	P691	V699	S499	M173	M173	MET	ASP	Y5
K1242	F1164	E1083	E985	E899	Y810	L693	T600	T600	R88	A174	LEU	TYR	E7
A1245	S1165	D1084	A986	E899	N811	R694	D601	V502	G89	R175	VAL	ILE	K8
R1246	D1166	P1086	K988	E899	A695	A695	E603	K503	G89	I176	PRO	ASP	K9
S1247	E1167	P1086	L989	L902	F812	D697	H604	F505	T91	P177	GLU	GLU	R10
S1250	E1168	Y1087	R894	I905	D814	T702	V605	Q510	A94	Y179	ARG	THR	I11
L1253	M1170	M1080	D995	F906	I816	G703	L606	M510	P95	R180	GLY	GLY	K12
V1254	L1171	I1096	TRP	G907	L817	M704	I609	M515	R101	R101	LEU	LEU	D14
T1255	L1172	I1097	LEU	E908	V818	E705	E610	V516	L184	D185	THR	THR	F15
Q1256	M1175	L1098	LEU	E908	S819	E705	E611	Q517	G16	F186	ALA	ALA	K17
P1258	L1176	L1099	LEU	K909	E820	V708	E611	N518	Y105	F187	ALA	ALA	K17
G1260	R1177	P1100	GLY	R821	R821	A709	Y614	M519	A109	F188	PHE	PHE	Q20
Q1265	Q1257	L1101	LEU	V822	V822	V710	V615	P520	F110	D189	ASP	ASP	V21
L1265	P1180	L1102	THR	R827	R827	V714	Q618	S522	M193	M193	ILE	ILE	Y26
L1269	P1181	G1102	ASP	F828	F828	T715	A619	E523	G112	G112	GLU	GLU	L27
G1261	V1185	L1103	GLU	S917	S917	T715	E524	I524	L27	L27	ALA	ALA	L27
K1262	V1186	S1105	GLU	L918	L918	Q725	L623	T525	L28	F195	ASN	ASN	L28
A1263	F1187	L1109	LYS	R919	R919	Q725	D624	H526	D83	V196	GLY	GLY	D83
G1265	F1187	I1109	GLN	N922	N922	V733	F629	K527	K37	I199	VAL	VAL	K37
F1265	L1188	G1110	ASN	G926	G926	I734	L633	R528	Q120	Q120	TYR	TYR	Q120
G1266	K1191	I1112	THR	T927	T927	I734	L633	R529	L194	L194	ALA	ALA	L27
F1267	E1192	L1113	GLU	V928	V928	D739	L633	L533	I39	I39	VAL	VAL	I39
Q1268	A1193	E1114	GLU	I929	I929	I748	R637	G534	E40	E40	LEU	LEU	E40
R1269	K1196	T1115	LYS	D930	D930	I748	S642	P535	Q41	Q41	GLY	GLY	Q41
F1270	L1197	H1116	GLN	T935	T935	D749	S642	L538	L129	L129	ARG	ARG	D42
E1272	L1198	A1120	ASN	E940	E940	L753	S646	L538	M130	M130	ARG	ARG	D42
Y1281	L1199	A1121	LEU	R941	R941	L753	S646	R542	T207	T207	ILE	ILE	E44
Q1288	K1200	T1037	THR	I880	I880	T757	D648	R542	L209	L209	THR	THR	E44
L1201	L1201	G1123	THR	T851	T851	R758	Q649	R548	G48	G48	ALA	ALA	Y47
G1202	G1202	I1124	THR	R852	R852	S759	V650	R548	V456	V456	ALA	ALA	G48
D1203	D1203	G1125	THR	R853	R853	N760	D651	R557	G457	G457	ARG	ARG	L49
L1204	L1204	D1126	THR	R854	R854	Q761	D651	V558	E458	E458	ILE	ILE	E50
P1205	G1045	D1126	THR	I854	I854	N762	D654	C559	M459	M459	ILE	ILE	A51
T1206	V1046	L946	THR	I854	I854	T763	D654	P560	M462	M462	GLN	GLN	A52
S1295	L1047	E947	THR	E947	E947	Q767	V660	I861	Q463	Q463	LEU	LEU	F53
V1298	K1048	I948	THR	I948	I948	M768	S662	P567	R470	R470	LEU	LEU	V56
V1298	L1212	M951	THR	M951	M951	L773	A665	L571	P345	P345	LYS	LYS	F57
R1301	G1215	D959	THR	D959	D959	D781	S666	L575	E349	E349	ASP	ASP	Q60
T1302	R1216	I966	THR	I966	I966	L791	P669	S576	L221	L221	ASP	ASP	F57
D1310	Q1146	L967	THR	L967	L967	G792	F670	V577	D222	D222	VAL	VAL	Q60
H1313	Q1220	R1147	THR	E968	E968	E793	G482	V577	L223	L223	VAL	VAL	S61
H1313	F1221	A1148	THR	E968	E968	L794	L671	A579	F224	F224	VAL	VAL	Y62
E1222	E1222	M1066	THR	L971	L971	A795	H673	G585	E225	E225	VAL	VAL	S63
V1225	V1225	L1151	THR	F972	F972	L796	H673	F586	F226	F226	PRO	PRO	G64
G1228	G1228	V1155	THR	R974	R974	L966	A683	L587	LYS	LYS	VAL	VAL	N65
											THR	THR	E67
											GLU	GLU	Y70
											ILE	ILE	Y73
											ALA	ALA	Y73
											ARG	ARG	R74
											ASP	ASP	R74



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma-54 factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	208.48Å 151.52Å 195.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 3.76 29.64 – 3.76	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.64-3.76) 98.1 (29.64-3.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.75Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.262 , 0.312 0.262 , 0.312	Depositor DCC
R_{free} test set	3078 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	143.4	Xtrriage
Anisotropy	0.735	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27004	wwPDB-VP
Average B, all atoms (Å ²)	178.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	G	0.17	0/2366	0.52	2/3215 (0.1%)
1	H	0.15	0/1637	0.41	2/2224 (0.1%)
2	I	0.18	1/9533 (0.0%)	0.47	4/12893 (0.0%)
3	J	0.17	1/10294 (0.0%)	0.42	1/13920 (0.0%)
4	K	0.13	0/622	0.40	0/838
5	M	0.22	0/2935	0.58	4/3989 (0.1%)
All	All	0.18	2/27387 (0.0%)	0.47	13/37079 (0.0%)

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	G	0	1
2	I	0	5
3	J	0	4
5	M	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	109	ALA	C-N	9.59	1.56	1.33
3	J	120	LEU	C-N	5.63	1.47	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	909	LYS	N-CA-C	8.54	120.59	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1154	ASP	N-CA-C	7.66	119.34	108.00
3	J	265	LEU	N-CA-C	-6.48	97.00	110.80
2	I	398	SER	CB-CA-C	-6.44	107.33	116.34
2	I	1154	ASP	CB-CA-C	-6.26	107.58	116.34

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	194	GLN	Peptide
2	I	1040	ASP	Peptide
2	I	1154	ASP	Peptide
2	I	1202	GLY	Peptide
2	I	889	PRO	Peptide

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	G	2337	0	2343	80	0
1	H	1619	0	1619	56	0
2	I	9382	0	9211	327	0
3	J	10148	0	10169	336	1
4	K	620	0	621	21	0
5	M	2895	0	2828	115	1
6	J	1	0	0	0	0
7	J	2	0	0	0	0
All	All	27004	0	26791	858	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 16.

The worst 5 of 858 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)
2:I:49:LEU:O	2:I:53:PHE:HB2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:LEU:O	1:G:47:LEU:HB2	1.74	0.88
5:M:216:ALA:HB1	5:M:253:ILE:HD11	1.56	0.87
3:J:289:ASP:O	3:J:293:ARG:HB2	1.77	0.84
5:M:127:GLN:HE22	5:M:182:ILE:HA	1.45	0.82

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)
3:J:82:GLY:O	5:M:438:SER:OG[3_745]	2.18	0.02

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	G	305/329 (93%)	270 (88%)	33 (11%)	2 (1%)	18	50
1	H	211/329 (64%)	191 (90%)	20 (10%)	0	100	100
2	I	1211/1342 (90%)	1094 (90%)	110 (9%)	7 (1%)	21	52
3	J	1326/1407 (94%)	1198 (90%)	125 (9%)	3 (0%)	43	72
4	K	77/91 (85%)	71 (92%)	6 (8%)	0	100	100
5	M	370/477 (78%)	345 (93%)	22 (6%)	3 (1%)	16	47
All	All	3500/3975 (88%)	3169 (90%)	316 (9%)	15 (0%)	30	61

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	166	SER
3	J	266	ASN
5	M	276	VAL
2	I	170	VAL

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Mol	Chain	Res	Type
2	I	437	ASN

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	G	252/286 (88%)	222 (88%)	30 (12%)	5	22
1	H	175/286 (61%)	155 (89%)	20 (11%)	5	23
2	I	999/1157 (86%)	865 (87%)	134 (13%)	4	19
3	J	1058/1168 (91%)	915 (86%)	143 (14%)	4	18
4	K	65/75 (87%)	55 (85%)	10 (15%)	2	15
5	M	306/423 (72%)	261 (85%)	45 (15%)	3	17
All	All	2855/3395 (84%)	2473 (87%)	382 (13%)	4	19

5 of 382 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	378	LYS
3	J	907	HIS
3	J	470	VAL
3	J	706	VAL
3	J	1079	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	27	GLN
5	M	127	GLN
5	M	352	GLN
2	I	834	GLN
2	I	832	HIS

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	309/329 (93%)	-0.32	2 (0%) 85 67	115, 174, 216, 248	0
1	H	215/329 (65%)	-0.26	1 (0%) 87 70	144, 209, 239, 261	0
2	I	1217/1342 (90%)	-0.29	6 (0%) 87 70	97, 179, 242, 273	0
3	J	1336/1407 (94%)	-0.31	4 (0%) 90 77	88, 182, 243, 270	0
4	K	79/91 (86%)	-0.51	0 100 100	131, 168, 207, 230	0
5	M	380/477 (79%)	-0.23	0 100 100	103, 150, 191, 226	0
All	All	3536/3975 (88%)	-0.30	13 (0%) 88 73	88, 177, 239, 273	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1334	GLY	3.3
3	J	1099	TYR	2.5
2	I	224	PHE	2.4
3	J	1110	GLU	2.4
1	G	39	LEU	2.4

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](#)

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. 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	B-factors(\AA^2)	Q<0.9
6	MG	J	1501	1/1	0.78	0.06	192,192,192,192	0
7	ZN	J	1502	1/1	0.98	0.10	225,225,225,225	0
7	ZN	J	1503	1/1	0.98	0.07	179,179,179,179	0

6.5 Other polymers [i](#)

There are no such residues in this entry.