



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2017 – 03:45 AM EDT

PDB ID : 4XMM  
Title : Structure of the yeast coat nucleoporin complex, space group C2  
Authors : Stuwe, T.; Correia, A.R.; Lin, D.H.; Paduch, M.; Lu, V.T.; Kossiakoff, A.A.;  
Hoelz, A.  
Deposited on : unknown  
Resolution : 7.38 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

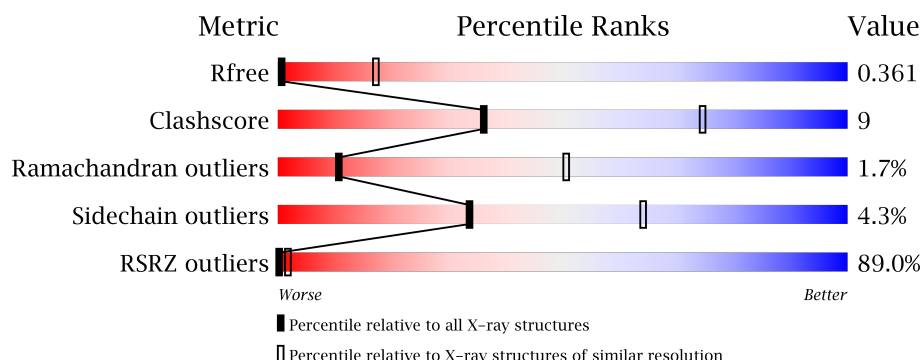
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 7.38 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))
$R_{free}$	100719	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)

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  $\geq 3$ , 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	297	<div> <div>92%</div> <div> <div>64%</div> <div>25%</div> <div>8%</div> </div> </div>
2	B	652	<div> <div>70%</div> <div> <div>56%</div> <div>19%</div> <div>22%</div> </div> </div>
3	C	349	<div> <div>83%</div> <div> <div>61%</div> <div>26%</div> <div>12%</div> </div> </div>
4	D	715	<div> <div>81%</div> <div> <div>66%</div> <div>19%</div> <div>13%</div> </div> </div>
5	E	1045	<div> <div>69%</div> <div> <div>71%</div> <div>14%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	F	454	<div><div>82%</div><div><div></div><div></div><div></div><div></div></div><div>68%21%•8%</div></div>
7	H	271	<div><div>70%</div><div><div></div><div></div><div></div><div></div></div><div>71%8%20%</div></div>
8	L	217	<div><div>85%</div><div><div></div><div></div><div></div><div></div></div><div>86%10%•</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26139 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	511	Total	C	N	O	S	0	0	0
			3805	2417	648	730	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MET	-	initiating methionine	UNP P49687
B	62	GLY	-	expression tag	UNP P49687
B	63	SER	-	expression tag	UNP P49687
B	64	SER	-	expression tag	UNP P49687
B	65	HIS	-	expression tag	UNP P49687
B	66	HIS	-	expression tag	UNP P49687
B	67	HIS	-	expression tag	UNP P49687
B	68	HIS	-	expression tag	UNP P49687
B	69	HIS	-	expression tag	UNP P49687
B	70	HIS	-	expression tag	UNP P49687
B	71	SER	-	expression tag	UNP P49687
B	72	ASP	-	expression tag	UNP P49687
B	73	GLN	-	expression tag	UNP P49687
B	74	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	307	Total	C	N	O	S	0	0	0
			2438	1543	422	462	11			

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	620	Total	C	N	O	S	0	0	0
			4535	2884	753	877	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	MET	-	initiating methionine	UNP P46673
D	31	GLY	-	expression tag	UNP P46673
D	32	SER	-	expression tag	UNP P46673
D	33	SER	-	expression tag	UNP P46673
D	34	HIS	-	expression tag	UNP P46673
D	35	HIS	-	expression tag	UNP P46673
D	36	HIS	-	expression tag	UNP P46673
D	37	HIS	-	expression tag	UNP P46673
D	38	HIS	-	expression tag	UNP P46673
D	39	HIS	-	expression tag	UNP P46673
D	40	SER	-	expression tag	UNP P46673
D	41	ASP	-	expression tag	UNP P46673
D	42	GLN	-	expression tag	UNP P46673
D	43	PRO	-	expression tag	UNP P46673

- Molecule 5 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	896	Total	C	N	O	S	0	0	0
			6622	4232	1099	1275	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	MET	-	initiating methionine	UNP P35729
E	-6	HIS	-	expression tag	UNP P35729
E	-5	HIS	-	expression tag	UNP P35729
E	-4	HIS	-	expression tag	UNP P35729
E	-3	HIS	-	expression tag	UNP P35729
E	-2	HIS	-	expression tag	UNP P35729
E	-1	HIS	-	expression tag	UNP P35729
E	0	SER	-	expression tag	UNP P35729
E	1	THR	-	expression tag	UNP P35729

- Molecule 6 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P52891
F	-1	PRO	-	expression tag	UNP P52891
F	0	HIS	-	expression tag	UNP P52891

- Molecule 7 is a protein called Antibody 57 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	217	Total	C	N	O	S	0	0	0
			1576	988	267	315	6			

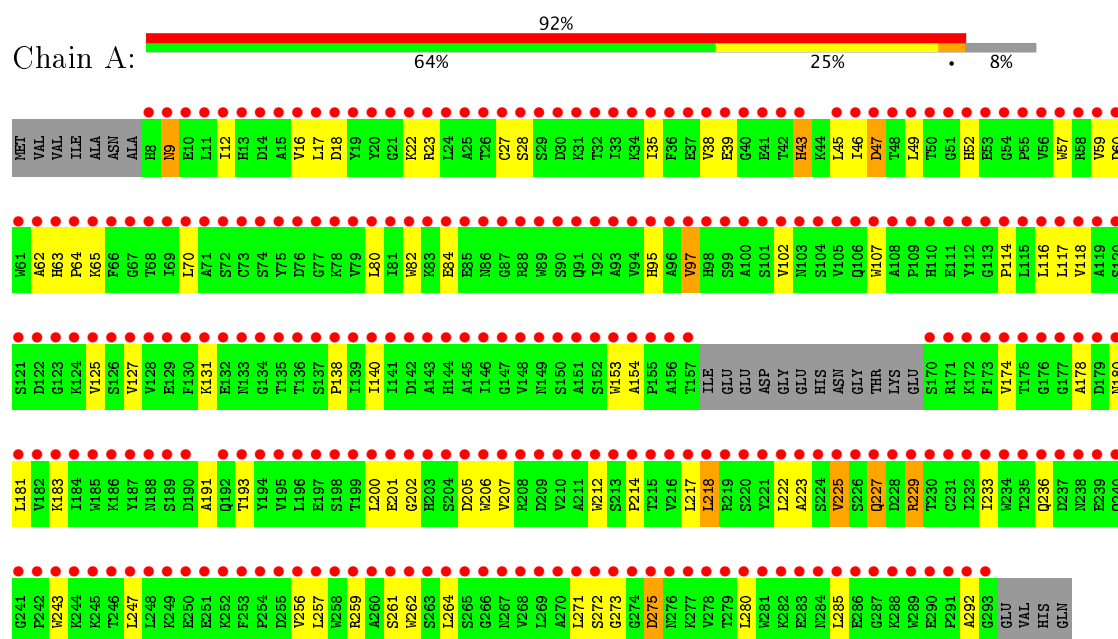
- Molecule 8 is a protein called Antibody 57 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	L	210	Total	C	N	O	S	0	0	0
			1599	996	270	327	6			

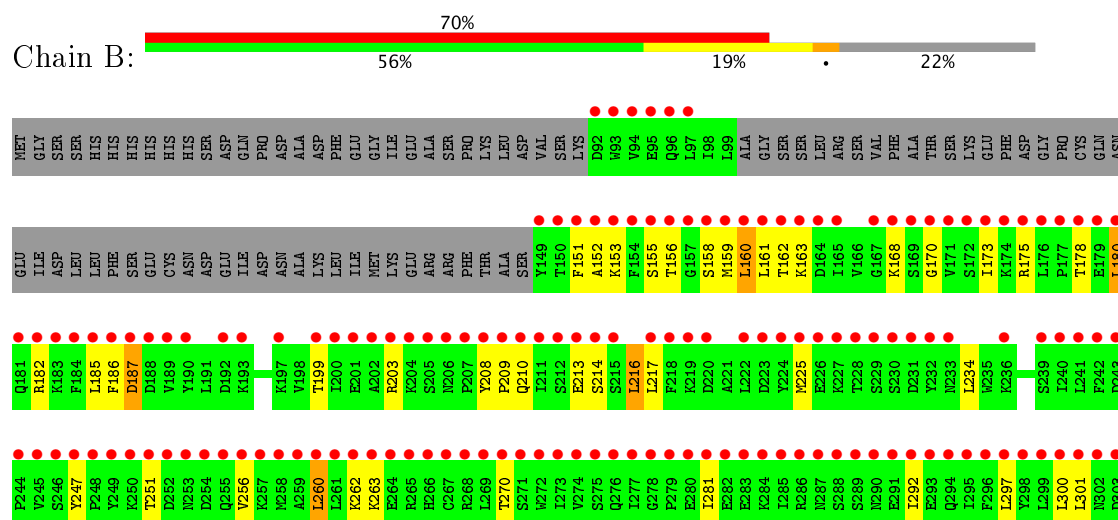
### 3 Residue-property plots

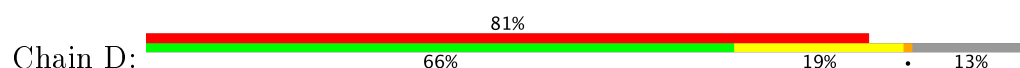
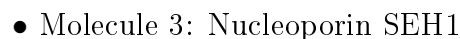
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Protein transport protein SEC13



#### • Molecule 2: Nucleoporin NUP145









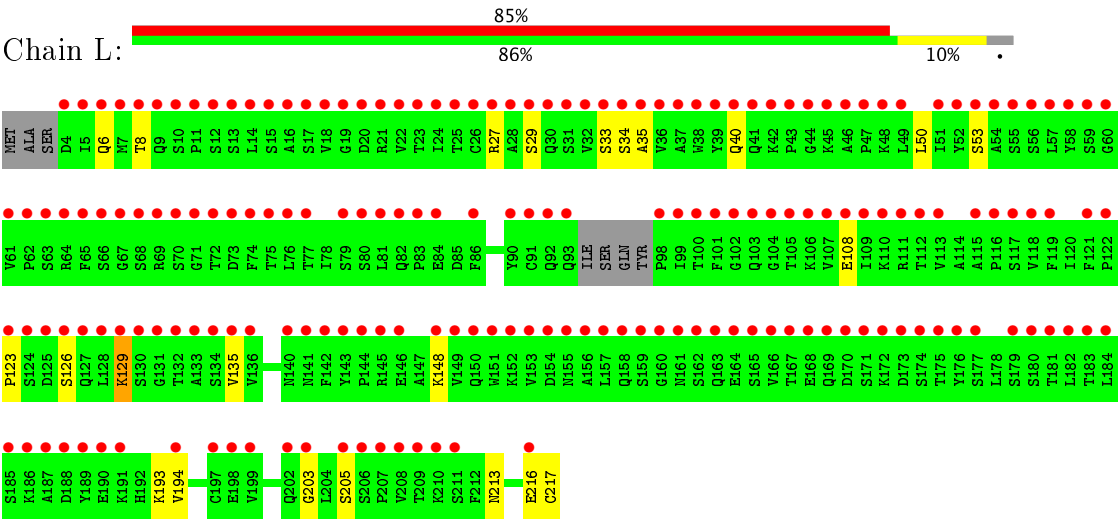
ILE	TRP	ASP	D833	F770	F710	E645	D585	L525	K454	D393	P320	T249	L183	V119
LEU	GLU	THR	ARG	D771	N711	I646	L586	R526	T455	D394	T321	S260	L184	
ASN		VAL	ASN	Q772	ALA	F647	I587	S527	A456	D395	N322	F251	G185	L123
SER			SER	S773	SER	G648	N588	I528	F457	D396	L323	T252	L186	
LYS			SER	Y774	ILE	Q649	N589	S529	N458	D397	S324	L253	K187	D126
VAL				Y775	T715	H650	O590	K331	N459	D398	A325	L254	K188	G125
V1025				E776	E716	I651	N591	F532	A460	D399	S326	Q255	Y189	S127
T1026				F777	N717	S652	K592	F533	S461	D400	A327	D256	D189	F128
T1027				F778	F718	T653	K593	D534	S462	D401	L328	Y257	G191	L129
T1028				H779	F719	L654	O594	D535	L463	D402	S329	D258	V192	T130
D1029				H780	D720	L655	I595	I535	T464	D403	K330	M259	H193	L131
I1030				H781	M721	D656	F596	I536	L465	V404	V335	V260	Y194	Q132
I1031				T782	T722	L657	N597	T537	Y466	E405	L336	Q262	F195	L133
R1032				P783	F723	H658	K598	G538	Y467	R406	L337	Q263	P196	P134
D1033				G784	F724	F659	K599	E539	D468	R407	T337	S264	L197	L135
L1034				R785	R725	K660	D600	L540	D469	F408	R338	O265	L198	L136
R1035				L786	F621	Q661	I602	P541	I470	O409	P339	S266	F199	F137
G1036				Y787	T726	F662	I603	D542	I471	N410	E341	D267	N200	L138
LEU				Y788	ILE	L663	S603	S543	N474	L411	E342	P268	D201	L139
				Y789	ILE	L664	A604	N544	C475	K412	L343	S269	N202	S140
				Y790	ILE	L665	L605	T545	F476	S413	N343	P270	S203	S141
				Y791	ASN	L666	K606	T546	Q477	R414	E344	F271	Y204	A142
				Y792	THR	L667	F607	V547	Y478	V415	E345	K272	L205	N143
				Y793	THR	Y668	D608	E548	Y479	O416	A346	V273	K206	T144
				Y794	THR	R669	O609	K549	M480	T417	S347	K274	S207	L145
				Y795	THR	Q670	F610	F550	V490	Q418	Y348	E274	G147	H146
				Y796	THR	D671	T611	T551	Y491	E421	I352	A275	R210	G148
				Y797	THR	K672	S612	D552	Y492	R422	W355	V276	F211	M149
				Y798	THR	C673	I613	I553	Y493	A423	K356	L280	F212	F150
				Y799	THR	L674	S615	K555	Y494	Q424	S357	Y283	S213	H151
				Y800	THR	L675	L616	N556	Y495	Q425	G358	N284	R214	L152
				Y801	THR	A676	B517	C557	Y496	L426	S359	N285	S215	Q153
				Y802	THR	E677	S618	L558	Y497	L427	T359	T286	N286	N154
				Y803	THR	V678	L619	E559	Y498	S428	A360	L287	K217	P155
				Y804	THR	L679	L619	N560	Y499	E429	S361	V288	S218	Y156
				Y805	THR	L680	H620	Q561	Y501	N430	K362	Y289	D219	D157
				Y806	THR	K681	O621	F562	Y502	K431	N369	L291	F220	F158
				Y807	THR	D682	L622	E563	Y503	L432	D370	P292	D221	T159
				Y808	THR	S683	L623	L564	Y504	L433	E371	L293	S222	V160
				Y809	THR	S684	S624	T565	Y505	N434	S372	E294	V223	R161
				Y810	THR	E685	L625	N566	Y506	A435	Y375	N295	L228	V162
				Y811	THR	F686	H626	L567	Y507	H436	N376	G296	F229	P163
				Y812	THR	S687	T627	K568	Y508	N437	Y377	L297	H230	H164
				Y813	THR	F688	R628	I569	Y509	E438	E378	M300	E231	F167
				Y814	THR	G689	L629	L570	Y510	D439	W379	Y305	R232	V169
				Y815	THR	V690	T630	F571	Y511	E440	I379	L304	Y233	S170
				Y816	THR	K691	L631	D572	Y512	E441	E380	ASP	P171	Q172
				Y817	THR	F692	O632	E573	Y513	Y442	S381	SER	F173	S174
				Y818	THR	F693	L633	L574	Y514	L443	K384	SER	N240	
				Y819	THR	N694	L634	N575	Y515	A444	S385	GLY	C241	
				Y820	THR	Y701	T636	N576	Y516	N445	V387	ILE	H242	F177
				Y821	THR	I702	L637	F577	Y517	N446	L386	ASP	L178	
				Y822	THR	D703	Y638	D578	Y518	E447	V388	SER	E279	
				Y823	THR	F704	N639	I579	Y519	T448	L389	GLY	D180	
				Y824	THR	S704	L640	P580	Y520	L449	Q390	ILE	I245	
				Y825	THR	L705	T640	V581	Y521	L450	T312	ASP	E246	
				Y826	THR	N706	D641	V582	Y522	R451	T313	ASP	G181	
				Y827	THR	S707	L642	V583	Y523	D452	T314	ASP	D247	
				Y828	THR	L708	D643	V584	Y524	V453	E392	TRP	L248	
				Y829	THR	V709	T644	N584	Y525					

• Molecule 6: Nucleoporin NUP84

Chain F:



● Molecule 8: Antibody 57 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.65Å 186.30Å 199.57Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	67.52 – 7.38 68.01 – 7.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (67.52-7.38) 99.7 (68.01-7.38)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 7.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1809)	Depositor
R, $R_{free}$	0.330 , 0.353 0.328 , 0.361	Depositor DCC
$R_{free}$ test set	1021 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	734.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.50 , -10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	26139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	716.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.32	0/2220	0.62	0/3028
2	B	0.37	0/3860	0.66	2/5224 (0.0%)
3	C	0.28	0/2499	0.64	0/3388
4	D	0.30	0/4602	0.58	2/6246 (0.0%)
5	E	0.33	0/6730	0.55	1/9158 (0.0%)
6	F	0.35	0/3472	0.64	2/4714 (0.0%)
7	H	0.31	0/1610	0.62	1/2194 (0.0%)
8	L	0.29	0/1631	0.60	0/2210
All	All	0.32	0/26624	0.60	8/36162 (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
2	B	0	2
5	E	0	2
6	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	167	GLY	N-CA-C	-6.40	97.09	113.10
4	D	608	PRO	N-CA-CB	6.10	110.62	103.30
2	B	187	ASP	CB-CG-OD2	6.04	123.73	118.30
7	H	219	LEU	CA-CB-CG	6.04	129.19	115.30
5	E	818	PRO	N-CA-CB	5.78	110.23	103.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	371	PHE	Peptide
2	B	392	TYR	Peptide
5	E	190	ASP	Mainchain
5	E	264	ASP	Sidechain
6	F	151	GLY	Mainchain

## 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	2160	0	2096	60	0
2	B	3805	0	3499	106	0
3	C	2438	0	2378	56	0
4	D	4535	0	4073	104	0
5	E	6622	0	5907	80	0
6	F	3404	0	3378	77	2
7	H	1576	0	1532	13	0
8	L	1599	0	1554	9	2
All	All	26139	0	24417	462	2

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 9.

The worst 5 of 462 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)
5:E:537:THR:HG22	5:E:743:ASN:HA	1.54	0.86
5:E:293:LEU:HD13	5:E:297:LEU:HD12	1.59	0.85
4:D:517:ASP:OD1	7:H:54:ASN:N	2.10	0.85
4:D:159:ILE:HG12	4:D:175:LEU:HB3	1.59	0.84
4:D:156:GLU:OE2	4:D:214:ARG:NH1	2.13	0.81

All (2) 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)
6:F:233:THR:OG1	8:L:203:GLY:O[4_455]	2.05	0.15
6:F:232:ASN:O	8:L:205:SER:N[4_455]	2.08	0.12

### 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	270/297 (91%)	228 (84%)	36 (13%)	6 (2%)	8	44
2	B	491/652 (75%)	451 (92%)	30 (6%)	10 (2%)	9	46
3	C	303/349 (87%)	266 (88%)	31 (10%)	6 (2%)	9	46
4	D	592/715 (83%)	532 (90%)	50 (8%)	10 (2%)	11	50
5	E	858/1045 (82%)	798 (93%)	49 (6%)	11 (1%)	14	56
6	F	413/454 (91%)	368 (89%)	34 (8%)	11 (3%)	6	40
7	H	213/271 (79%)	206 (97%)	7 (3%)	0	100	100
8	L	206/217 (95%)	198 (96%)	6 (3%)	2 (1%)	18	61
All	All	3346/4000 (84%)	3047 (91%)	243 (7%)	56 (2%)	11	50

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	SER
2	B	368	GLU
2	B	371	PHE
2	B	394	GLN
3	C	43	SER

#### 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	233/252 (92%)	224 (96%)	9 (4%)	37	66
2	B	367/594 (62%)	332 (90%)	35 (10%)	10	36
3	C	269/305 (88%)	261 (97%)	8 (3%)	46	72
4	D	424/642 (66%)	414 (98%)	10 (2%)	54	78
5	E	639/980 (65%)	616 (96%)	23 (4%)	40	68
6	F	387/418 (93%)	367 (95%)	20 (5%)	27	59
7	H	175/224 (78%)	170 (97%)	5 (3%)	48	73
8	L	184/191 (96%)	179 (97%)	5 (3%)	50	74
All	All	2678/3606 (74%)	2563 (96%)	115 (4%)	33	64

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	51	MET
5	E	127	SER
7	H	113	ARG
4	D	143	THR
4	D	488	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	313	ASN
4	D	467	ASN
5	E	575	ASN
2	B	542	GLN
5	E	588	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 [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	274/297 (92%)	15.07	272 (99%) 0 1	629, 712, 763, 800	0
2	B	511/652 (78%)	9.33	459 (89%) 0 2	374, 655, 746, 784	0
3	C	307/349 (87%)	10.24	290 (94%) 0 1	631, 756, 814, 905	0
4	D	620/715 (86%)	9.98	581 (93%) 0 1	388, 746, 989, 1000	0
5	E	896/1045 (85%)	8.87	726 (81%) 0 2	422, 725, 816, 883	0
6	F	419/454 (92%)	12.15	373 (89%) 0 2	545, 699, 803, 877	0
7	H	217/271 (80%)	8.87	189 (87%) 0 2	528, 677, 821, 884	0
8	L	210/217 (96%)	8.38	185 (88%) 0 2	526, 676, 756, 791	0
All	All	3454/4000 (86%)	10.12	3075 (89%) 0 2	374, 711, 890, 1000	0

The worst 5 of 3075 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ASP	75.7
5	E	519	THR	62.9
1	A	27	CYS	59.4
1	A	100	ALA	58.7
2	B	153	LYS	56.3

### 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 ⓘ

There are no carbohydrates 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.