



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2017 – 05:52 AM EDT

PDB ID : 3DIN
Title : Crystal structure of the protein-translocation complex formed by the SecY channel and the SecA ATPase
Authors : Zimmer, J.; Nam, Y.; Rapoport, T.A.
Deposited on : unknown
Resolution : 4.50 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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-20030345

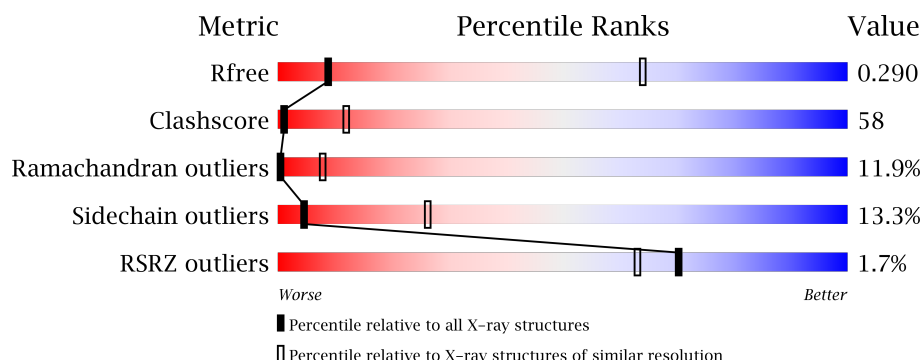
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1007 (5.30-3.64)
Clashscore	112137	1029 (5.30-3.70)
Ramachandran outliers	110173	1025 (5.30-3.66)
Sidechain outliers	110143	1006 (5.30-3.66)
RSRZ outliers	101464	1015 (5.30-3.64)

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	871	<div> <div>21% 55% 17% 6%</div> </div>
1	B	871	<div> <div>21% 54% 17% 6%</div> </div>
2	C	431	<div> <div>3% 27% 50% 13% 8%</div> </div>
2	F	431	<div> <div>2% 27% 51% 12% 8%</div> </div>
3	D	65	<div> <div>32% 51% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	65	
4	E	76	
4	H	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ADP	A	873	-	-	X	-
6	ADP	B	873	-	-	X	-
7	BEF	A	874	-	-	X	-
7	BEF	B	874	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21368 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 translocase subunit secA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	816	Total	C	N	O	S	0	0	0
			6613	4215	1131	1239	28			
1	B	816	Total	C	N	O	S	0	0	0
			6613	4215	1131	1239	28			

- Molecule 2 is a protein called Preprotein translocase subunit SecY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	396	Total	C	N	O	S	0	0	0
			3124	2071	518	524	11			
2	F	396	Total	C	N	O	S	0	0	0
			3124	2071	518	524	11			

- Molecule 3 is a protein called Preprotein translocase subunit secE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	56	Total	C	N	O	0	0	0
			431	294	64	73			
3	G	56	Total	C	N	O	0	0	0
			431	294	64	73			

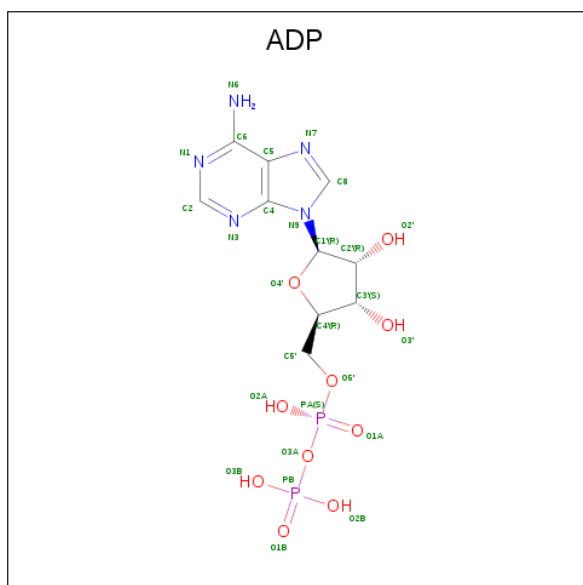
- Molecule 4 is a protein called Preprotein translocase subunit SecG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	65	Total	C	N	O	S	0	0	0
			484	318	80	83	3			
4	H	65	Total	C	N	O	S	0	0	0
			484	318	80	83	3			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

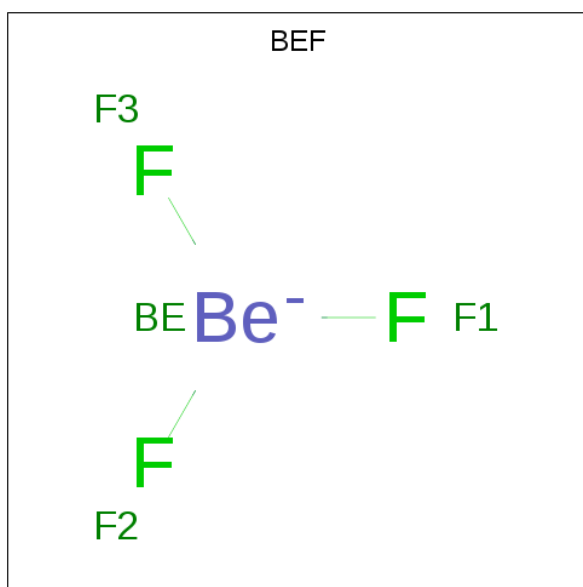
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

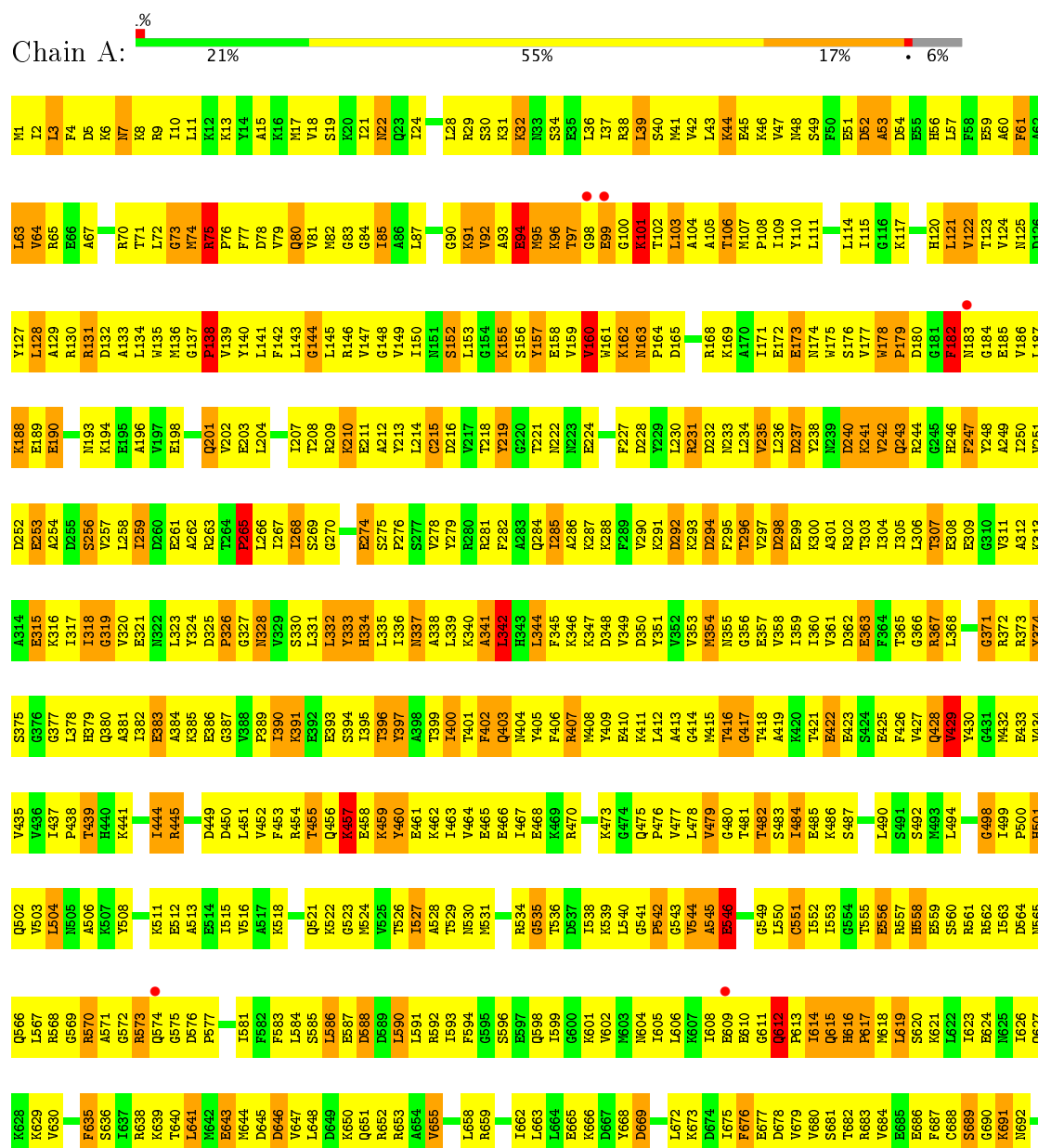


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Be	F	0	0
			4	1	3		
7	B	1	Total	Be	F	0	0
			4	1	3		

3 Residue-property plots

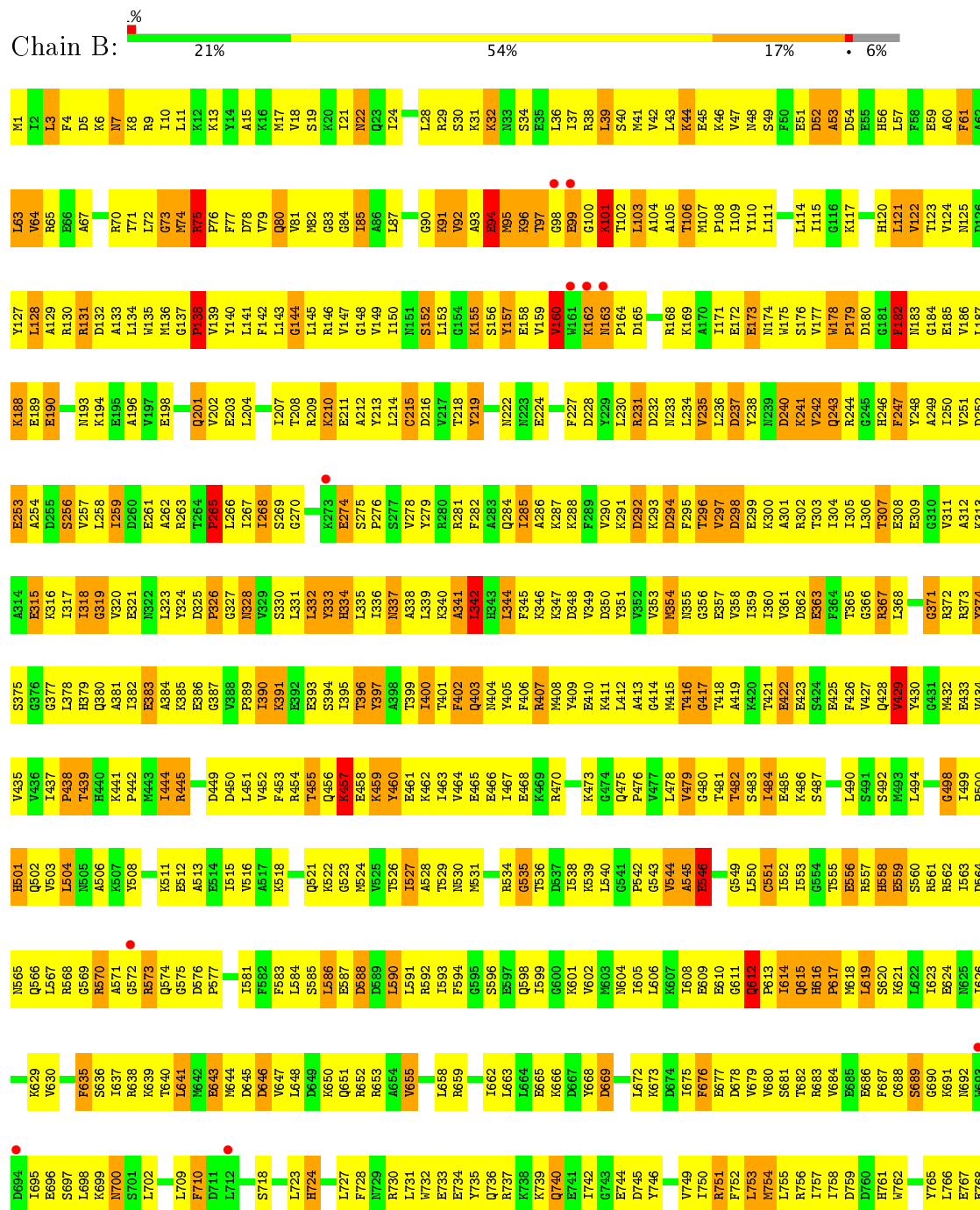
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

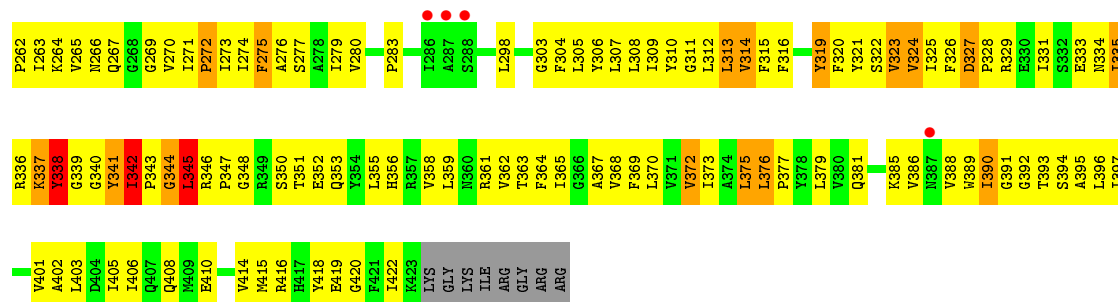
- Molecule 1: Protein translocase subunit secA



ILE	ARG	LEU	VAL	HIS	GLU	GLU	PHE	ASN	LEU	VAL	ASN	ARG	ALA	MET	ARG	ARG	ALA	THR	GLU	LYS	LYS	LYS	ASP	GLY	LEU	HIS	SER	PHE	GLY	ARG	ILE	ARG	VAL	LYS	VAL	LYS	VAL	SER	GLU	LYS	ASP	GLU	LYS	ALA	GLU	GLU	LYS	GLY	LYS							
H771	H772	K773	E774	H775	H776	H777	H778	H779	H780	Q783	K784	D785	H786	I787	H788	E789	F790	F791	K792	E793	T794	M797	F798	M801	K802	R803	R804	I805	D806	D807	T808	I809	D810	H811	H812	V813	I814	R815	V816	VAL	LYS	VAL	LYS	SER	GLU	LYS	ASP	GLU	LYS	ALA	LYS	GLU	GLU	LYS	GLY	LYS
L695	E696	S697	L698	K699	H700	S701	L702	L709	F710	S718	L723	H724	L727	F728	H729	R730	L731	H732	E734	F735	Q736	R737	K738	K739	Q740	E741	I742	G743	E744	D745	V746	R747	K748	V749	L750	R751	F752	L753	M754	L755	R756	I757	L758	D759	D760	H761	H762	Y765	L766	E767	E768	V769	E770			

• Molecule 1: Protein translocase subunit secA





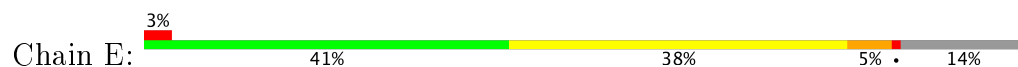
• Molecule 3: Preprotein translocase subunit secE



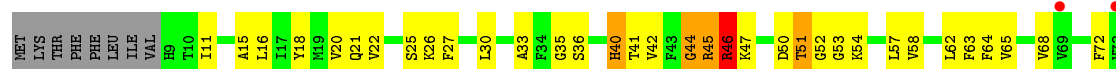
• Molecule 3: Preprotein translocase subunit secE



• Molecule 4: Preprotein translocase subunit SecG



• Molecule 4: Preprotein translocase subunit SecG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.62Å 156.00Å 358.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 4.50 19.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (15.00-4.50) 97.2 (19.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 4.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.303 0.291 , 0.290	Depositor DCC
R_{free} test set	1652 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	205.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 255.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21368	wwPDB-VP
Average B, all atoms (Å ²)	356.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, BEF, ADP

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	0.31	0/6730	0.62	1/9048 (0.0%)
1	B	0.31	0/6730	0.62	1/9048 (0.0%)
2	C	0.44	1/3194 (0.0%)	0.68	1/4329 (0.0%)
2	F	0.42	0/3194	0.69	2/4329 (0.0%)
3	D	0.32	0/440	0.54	0/596
3	G	0.33	0/440	0.54	0/596
4	E	0.31	0/492	0.55	0/662
4	H	0.31	0/492	0.55	0/662
All	All	0.35	1/21712 (0.0%)	0.63	5/29270 (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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	235	GLN	N-CA	5.64	1.57	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	236	ALA	N-CA-C	5.62	126.17	111.00
2	F	228	PHE	CB-CG-CD1	5.53	124.67	120.80
2	C	236	ALA	N-CA-C	5.37	125.50	111.00
1	A	94	GLU	CB-CA-C	-5.18	100.04	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	GLU	CB-CA-C	-5.18	100.05	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	260	TYR	Sidechain

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	6613	0	6689	906	2
1	B	6613	0	6689	891	2
2	C	3124	0	3275	347	0
2	F	3124	0	3275	336	0
3	D	431	0	460	29	0
3	G	431	0	460	33	0
4	E	484	0	508	29	0
4	H	484	0	508	28	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	12	40	0
6	B	27	0	12	38	0
7	A	4	0	0	4	0
7	B	4	0	0	5	0
All	All	21368	0	21888	2490	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 58.

The worst 5 of 2490 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:76:PRO:HD2	6:A:873:ADP:N6	1.34	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PRO:CD	6:A:873:ADP:HN62	1.40	1.34
1:B:76:PRO:HD2	6:B:873:ADP:N6	1.45	1.30
1:B:76:PRO:CD	6:B:873:ADP:HN62	1.50	1.25
1:B:101:LYS:HE2	7:B:874:BEF:F2	1.31	1.21

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)
1:A:498:GLY:O	1:B:518:LYS:NZ[1_455]	2.07	0.13
1:A:518:LYS:NZ	1:B:498:GLY:O[1_455]	2.17	0.03

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	814/871 (94%)	510 (63%)	207 (25%)	97 (12%)	0	8
1	B	814/871 (94%)	511 (63%)	206 (25%)	97 (12%)	0	8
2	C	392/431 (91%)	260 (66%)	80 (20%)	52 (13%)	0	6
2	F	392/431 (91%)	262 (67%)	78 (20%)	52 (13%)	0	6
3	D	54/65 (83%)	41 (76%)	9 (17%)	4 (7%)	1	19
3	G	54/65 (83%)	41 (76%)	9 (17%)	4 (7%)	1	19
4	E	63/76 (83%)	46 (73%)	12 (19%)	5 (8%)	1	18
4	H	63/76 (83%)	46 (73%)	12 (19%)	5 (8%)	1	18
All	All	2646/2886 (92%)	1717 (65%)	613 (23%)	316 (12%)	0	8

5 of 316 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	95	MET
1	A	131	ARG
1	A	152	SER
1	A	178	TRP

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	717/766 (94%)	610 (85%)	107 (15%)	3	22
1	B	717/766 (94%)	610 (85%)	107 (15%)	3	22
2	C	331/356 (93%)	293 (88%)	38 (12%)	6	31
2	F	331/356 (93%)	294 (89%)	37 (11%)	7	32
3	D	47/56 (84%)	44 (94%)	3 (6%)	20	54
3	G	47/56 (84%)	44 (94%)	3 (6%)	20	54
4	E	53/64 (83%)	48 (91%)	5 (9%)	10	39
4	H	53/64 (83%)	48 (91%)	5 (9%)	10	39
All	All	2296/2484 (92%)	1991 (87%)	305 (13%)	4	26

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	327	ASP
1	B	122	VAL
2	F	232	LEU
2	C	372	VAL
1	B	22	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	353	GLN

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Mol	Chain	Res	Type
1	B	112	ASN
2	F	143	ASN
2	C	360	ASN
1	B	22	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
6	ADP	A	873	7	25,29,29	1.56	4 (16%)	24,45,45	1.98	3 (12%)
7	BEF	A	874	6	0,3,3	0.00	-	0,3,3	0.00	-
6	ADP	B	873	7	25,29,29	1.56	4 (16%)	24,45,45	1.98	3 (12%)
7	BEF	B	874	6	0,3,3	0.00	-	0,3,3	0.00	-

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
6	ADP	A	873	7	-	0/12/32/32	0/3/3/3
7	BEF	A	874	6	-	0/0/0/0	0/0/0/0
6	ADP	B	873	7	-	0/12/32/32	0/3/3/3
7	BEF	B	874	6	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	873	ADP	C2-N3	2.05	1.35	1.32
6	B	873	ADP	C2-N3	2.07	1.35	1.32
6	B	873	ADP	PB-O1B	2.08	1.57	1.50
6	A	873	ADP	PB-O1B	2.09	1.57	1.50
6	A	873	ADP	PB-O3A	2.62	1.64	1.60

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	873	ADP	N3-C2-N1	-7.75	122.11	128.86
6	A	873	ADP	N3-C2-N1	-7.72	122.13	128.86
6	B	873	ADP	C1'-N9-C4	-2.72	121.94	126.64
6	A	873	ADP	C1'-N9-C4	-2.71	121.96	126.64
6	B	873	ADP	O3B-PB-O2B	2.36	117.15	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	873	ADP	40	0
7	A	874	BEF	4	0
6	B	873	ADP	38	0
7	B	874	BEF	5	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	816/871 (93%)	-0.50	5 (0%) 89 85	108, 306, 457, 500	0
1	B	816/871 (93%)	-0.46	10 (1%) 79 72	108, 306, 457, 500	0
2	C	396/431 (91%)	-0.14	15 (3%) 41 34	223, 429, 500, 500	0
2	F	396/431 (91%)	-0.19	10 (2%) 58 49	223, 429, 500, 500	0
3	D	56/65 (86%)	-0.44	0 100 100	322, 414, 500, 500	0
3	G	56/65 (86%)	-0.44	2 (3%) 43 36	322, 414, 500, 500	0
4	E	65/76 (85%)	-0.07	2 (3%) 49 41	326, 444, 490, 500	0
4	H	65/76 (85%)	-0.11	2 (3%) 49 41	326, 444, 490, 500	0
All	All	2666/2886 (92%)	-0.37	46 (1%) 70 63	108, 365, 489, 500	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	LYS	5.6
2	C	69	GLY	5.2
1	A	98	GLY	5.1
1	B	572	GLY	4.9
2	C	197	ALA	4.6

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](#)

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
6	ADP	A	873	27/27	0.69	0.34	-0.52	134,186,192,399	0
5	MG	A	872	1/1	0.90	0.30	-0.58	130,130,130,130	0
6	ADP	B	873	27/27	0.79	0.27	-0.89	134,186,192,399	0
7	BEF	A	874	4/4	0.64	0.30	-0.90	112,134,154,241	0
7	BEF	B	874	4/4	0.85	0.21	-0.97	112,134,154,241	0
5	MG	B	872	1/1	0.90	0.17	-1.14	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.