



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 11:28 PM EST

PDB ID : 5EUL
Title : Structure of the SecA-SecY complex with a translocating polypeptide substrate
Authors : Li, L.; Park, E.; Ling, J.; Ingram, J.; Ploegh, H.; Rapoport, T.A.
Deposited on : 2015-11-18
Resolution : 3.70 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

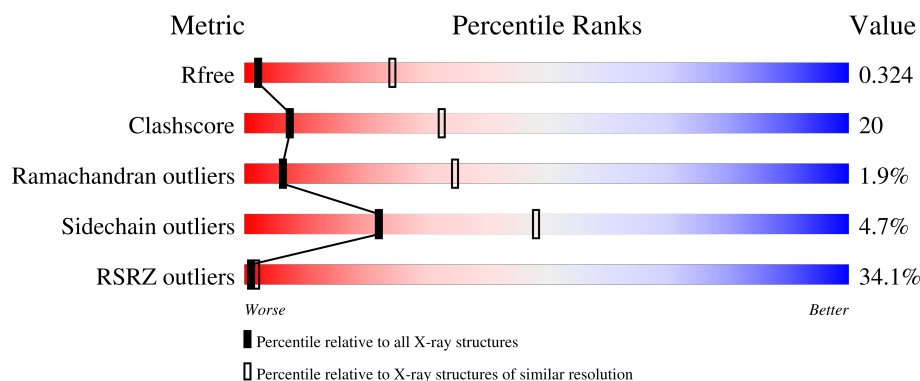
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	836	<div> <div>31%</div> <div>60%</div> <div>25%</div> <div>• •</div> <div>11%</div> </div>
2	Y	424	<div> <div>33%</div> <div>49%</div> <div>35%</div> <div>• •</div> <div>10%</div> </div>
3	E	70	<div> <div>19%</div> <div>56%</div> <div>23%</div> <div>•</div> <div>20%</div> </div>
4	V	131	<div> <div>25%</div> <div>54%</div> <div>29%</div> <div>• •</div> <div>12%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	TBR	A	1014	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10511 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, Insertion Peptide Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	746	Total	C	N	O	S	0	0	0
			5876	3677	1030	1135	34			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	828	THR	-	expression tag	UNP P28366
A	829	SER	-	expression tag	UNP P28366
A	830	LEU	-	expression tag	UNP P28366
A	831	GLU	-	expression tag	UNP P28366
A	832	VAL	-	expression tag	UNP P28366
A	833	LEU	-	expression tag	UNP P28366
A	834	PHE	-	expression tag	UNP P28366
A	835	GLN	-	expression tag	UNP P28366
A	836	GLY	-	expression tag	UNP P28366

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	380	Total	C	N	O	S	0	0	0
			2936	1951	478	495	12			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	60	CYS	GLY	conflict	UNP A4IJK8
Y	208	THR	GLN	conflict	UNP A4IJK8
Y	?	-	GLU	deletion	UNP A4IJK8
Y	?	-	ASN	deletion	UNP A4IJK8
Y	?	-	VAL	deletion	UNP A4IJK8
Y	?	-	GLY	deletion	UNP A4IJK8
Y	?	-	GLU	deletion	UNP A4IJK8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	?	-	ASP	deletion	UNP A4IJK8
Y	210	GLY	LEU	conflict	UNP A4IJK8
Y	211	GLY	PHE	conflict	UNP A4IJK8
Y	213	ASN	ARG	conflict	UNP A4IJK8

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	56	Total	C	N	O	0	0	0
			460	306	78	76			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLY	-	expression tag	UNP A4IJH4
E	62	GLY	-	expression tag	UNP A4IJH4
E	63	HIS	-	expression tag	UNP A4IJH4
E	64	HIS	-	expression tag	UNP A4IJH4
E	65	HIS	-	expression tag	UNP A4IJH4
E	66	HIS	-	expression tag	UNP A4IJH4
E	67	HIS	-	expression tag	UNP A4IJH4
E	68	HIS	-	expression tag	UNP A4IJH4
E	69	HIS	-	expression tag	UNP A4IJH4
E	70	HIS	-	expression tag	UNP A4IJH4

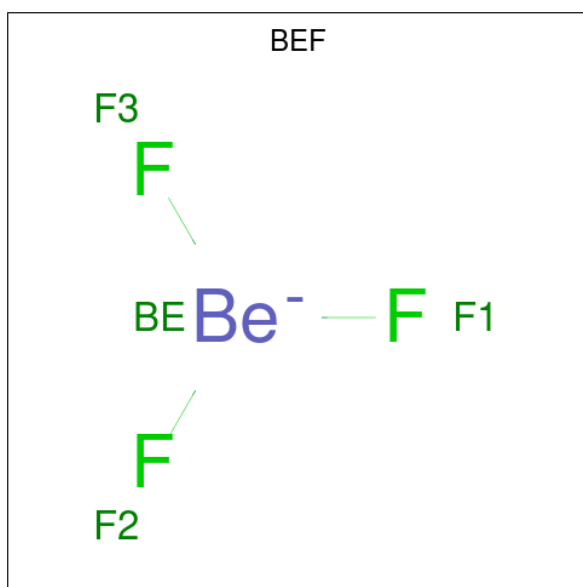
- Molecule 4 is a protein called AYC08.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	V	115	Total	C	N	O	S	0	0	0
			883	553	153	171	6			

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

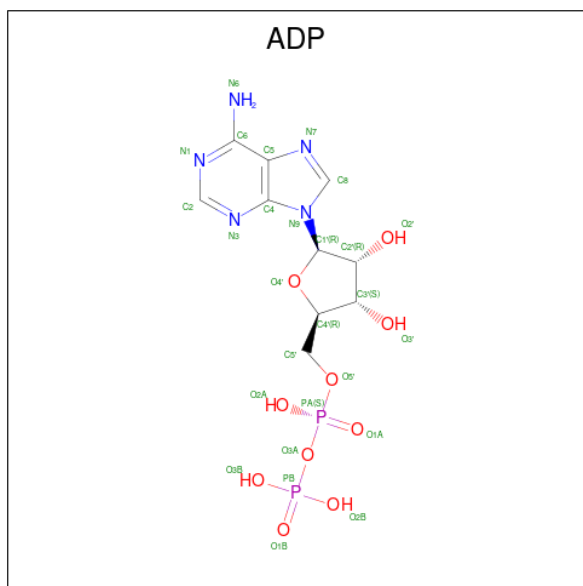
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



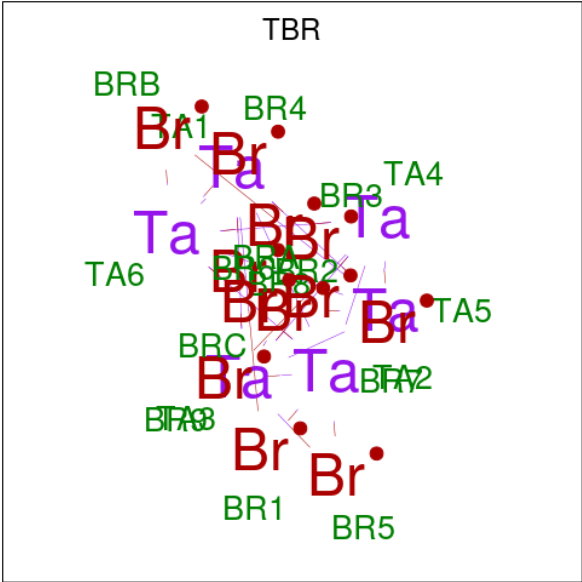
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	Be	F		0	0
			4	1	3			

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 8 is HEXATANTALUM DODECABROMIDE (three-letter code: TBR) (formula: $Br_{12}Ta_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		
8	A	1	Total	Br	Ta	0	0
			18	12	6		

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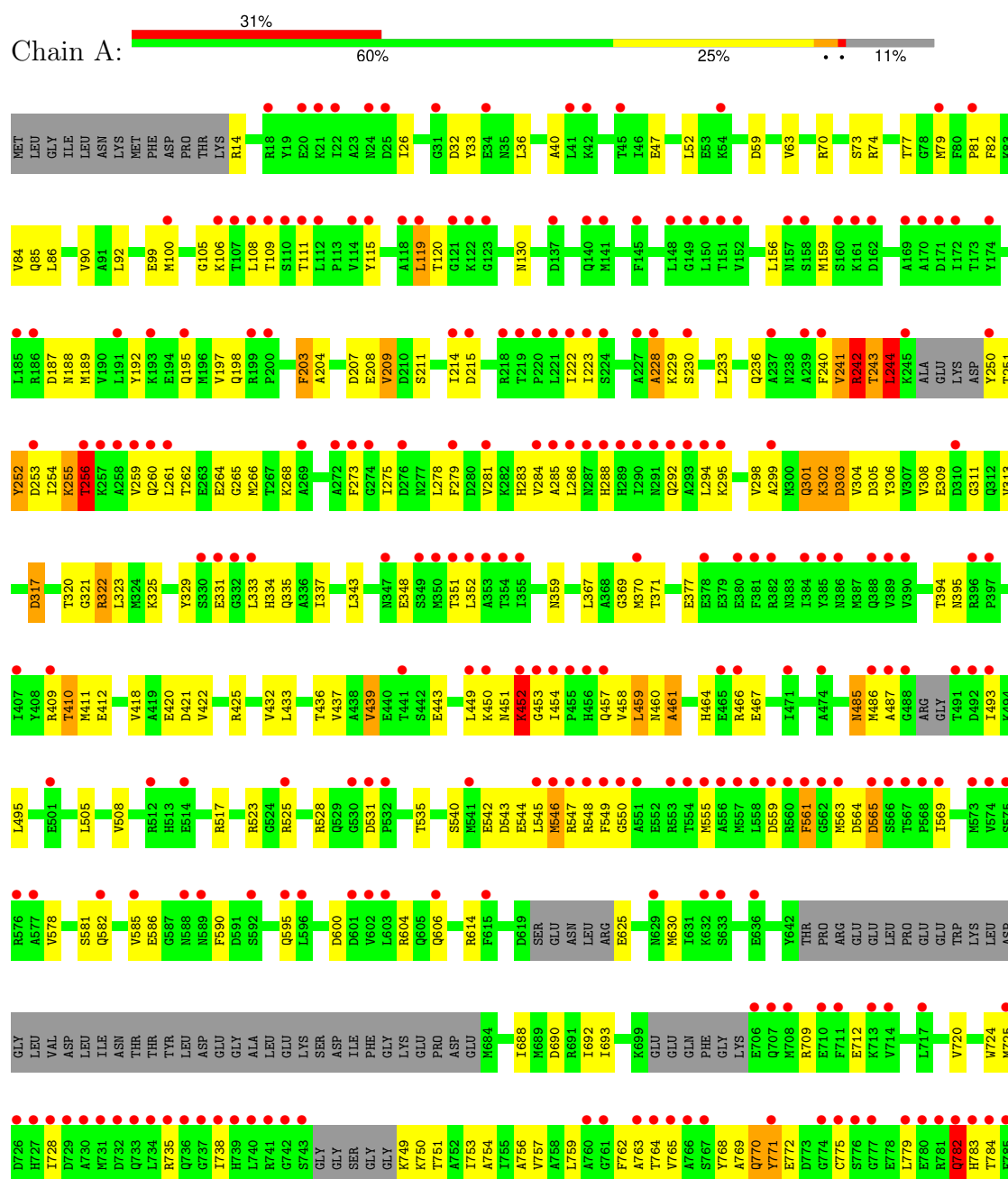
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0
8	Y	1	Total 18	Br 12	Ta 6	0	0

3 Residue-property plots

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. 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. 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, Insertion Peptide Chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.80Å 127.80Å 554.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.85 – 3.70 53.85 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.85-3.70) 99.9 (53.85-3.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.295 , 0.315 0.299 , 0.324	Depositor DCC
R_{free} test set	1513 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	191.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 96.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	10511	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, TBR, MG, 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	0.29	1/5950 (0.0%)	0.55	2/7993 (0.0%)
2	Y	0.37	0/2996	0.68	3/4069 (0.1%)
3	E	0.31	0/469	0.52	0/635
4	V	0.29	0/901	0.67	1/1222 (0.1%)
All	All	0.32	1/10316 (0.0%)	0.60	6/13919 (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	A	0	14
2	Y	0	8
4	V	0	3
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	804	PHE	CB-CG	-5.07	1.42	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	46	LEU	CA-CB-CG	7.64	132.87	115.30
4	V	43	LYS	N-CA-C	6.37	128.19	111.00
1	A	804	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	A	256	THR	N-CA-C	5.74	126.50	111.00
2	Y	89	MET	C-N-CA	5.55	135.59	121.70

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ALA	Peptide
1	A	229	LYS	Peptide
1	A	242	ARG	Peptide
1	A	243	THR	Peptide
1	A	244	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	5876	0	5855	215	0
2	Y	2936	0	3075	187	0
3	E	460	0	482	26	0
4	V	883	0	845	38	0
5	A	1	0	0	0	0
6	A	4	0	0	1	0
7	A	27	0	12	1	0
8	A	270	0	0	28	0
8	Y	54	0	0	2	0
All	All	10511	0	10269	416	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 20.

The worst 5 of 416 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:Y:265:LYS:HG3	2:Y:266:VAL:HG23	1.42	1.00
1:A:242:ARG:HH22	1:A:268:LYS:HB3	1.30	0.94
2:Y:229:VAL:HG12	3:E:30:THR:HG21	1.52	0.92
2:Y:24:MET:HB3	2:Y:166:LEU:HD21	1.51	0.90
2:Y:235:GLN:HG3	2:Y:266:VAL:HG22	1.55	0.88

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	730/836 (87%)	676 (93%)	42 (6%)	12 (2%)	8	37
2	Y	368/424 (87%)	335 (91%)	24 (6%)	9 (2%)	5	30
3	E	54/70 (77%)	49 (91%)	4 (7%)	1 (2%)	6	35
4	V	111/131 (85%)	99 (89%)	10 (9%)	2 (2%)	7	35
All	All	1263/1461 (86%)	1159 (92%)	80 (6%)	24 (2%)	6	35

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	THR
1	A	411	MET
1	A	452	LYS
1	A	782	GLN
1	A	783	HIS

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	622/706 (88%)	598 (96%)	24 (4%)	27	53
2	Y	313/354 (88%)	293 (94%)	20 (6%)	14	42
3	E	50/63 (79%)	48 (96%)	2 (4%)	27	52
4	V	93/108 (86%)	88 (95%)	5 (5%)	18	46
All	All	1078/1231 (88%)	1027 (95%)	51 (5%)	22	48

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Y	45	LYS
2	Y	199	TYR
4	V	99	ARG
2	Y	46	LEU
2	Y	83	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	101	GLN
2	Y	169	GLN
4	V	13	GLN
2	Y	308	HIS
2	Y	134	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	BEF	A	1002	7	0,3,3	-	-	-		
8	TBR	Y	502	-	0,36,36	-	-	-		
8	TBR	A	1016	-	0,36,36	-	-	-		
8	TBR	A	1006	-	0,36,36	-	-	-		
8	TBR	A	1009	-	0,36,36	-	-	-		
7	ADP	A	1003	6,5	24,29,29	0.93	1 (4%)	29,45,45	1.28	2 (6%)
8	TBR	A	1007	-	0,36,36	-	-	-		
8	TBR	A	1010	-	0,36,36	-	-	-		
8	TBR	A	1013	-	0,36,36	-	-	-		
8	TBR	A	1008	-	0,36,36	-	-	-		
8	TBR	A	1011	-	0,36,36	-	-	-		
8	TBR	A	1005	-	0,36,36	-	-	-		
8	TBR	A	1018	-	0,36,36	-	-	-		
8	TBR	A	1015	-	0,36,36	-	-	-		
8	TBR	A	1004	-	0,36,36	-	-	-		
8	TBR	A	1012	-	0,36,36	-	-	-		
8	TBR	Y	503	-	0,36,36	-	-	-		
8	TBR	Y	501	-	0,36,36	-	-	-		
8	TBR	A	1017	-	0,36,36	-	-	-		
8	TBR	A	1014	-	0,36,36	-	-	-		

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
7	ADP	A	1003	6,5	-	3/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1003	ADP	PA-O3A	2.15	1.61	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1003	ADP	N3-C2-N1	-3.66	123.71	128.67
7	A	1003	ADP	C4-C5-N7	-2.61	106.58	109.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

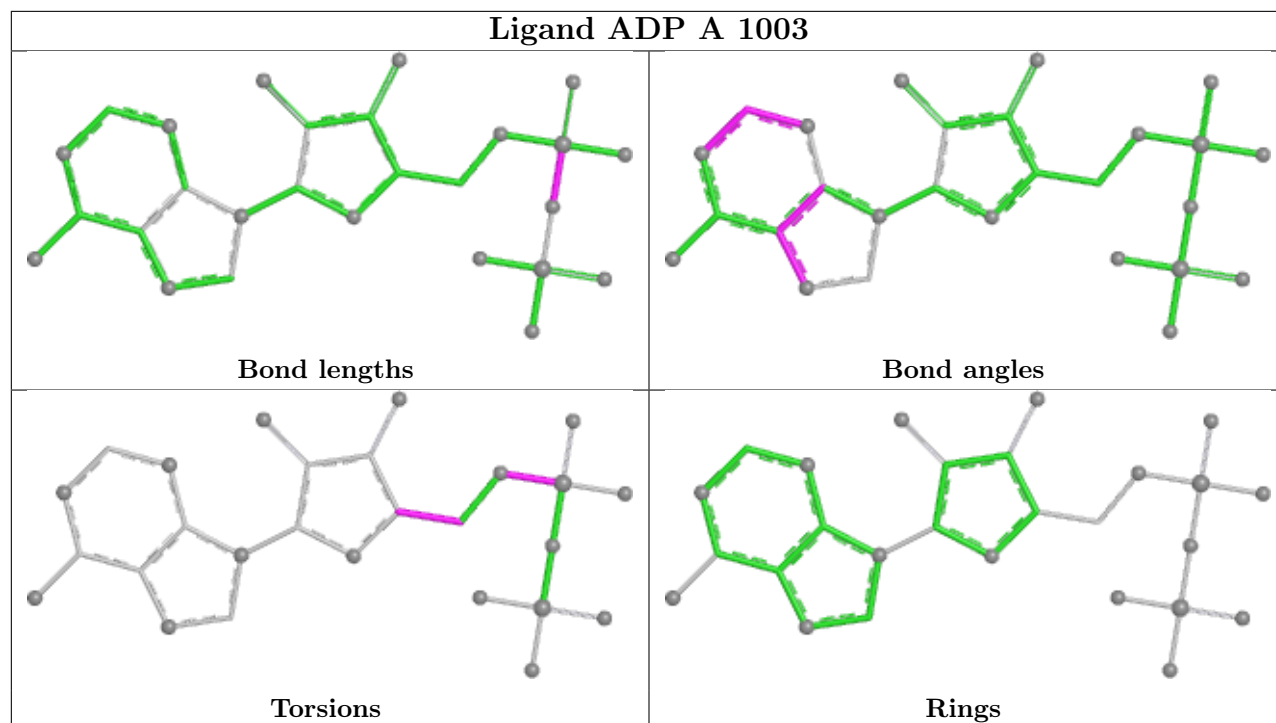
Mol	Chain	Res	Type	Atoms
7	A	1003	ADP	C5'-O5'-PA-O1A
7	A	1003	ADP	C5'-O5'-PA-O2A
7	A	1003	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

18 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	BEF	1	0
8	Y	502	TBR	2	0
8	A	1016	TBR	1	0
8	A	1006	TBR	2	0
8	A	1009	TBR	1	0
7	A	1003	ADP	1	0
8	A	1007	TBR	2	0
8	A	1010	TBR	3	0
8	A	1013	TBR	2	0
8	A	1008	TBR	1	0
8	A	1011	TBR	1	0
8	A	1005	TBR	1	0
8	A	1018	TBR	1	0
8	A	1015	TBR	3	0
8	A	1004	TBR	1	0
8	A	1012	TBR	2	0
8	A	1017	TBR	2	0
8	A	1014	TBR	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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](#)

Warning: The R factor obtained from EDS is 0.3527, which does not match the depositor's R factor of 0.2952. Please interpret the results in this section carefully.

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	746/836 (89%)	2.32	257 (34%) 1 2	113, 202, 268, 329	0
2	Y	380/424 (89%)	2.53	139 (36%) 1 1	116, 191, 258, 282	0
3	E	56/70 (80%)	1.10	13 (23%) 2 4	155, 220, 261, 265	0
4	V	115/131 (87%)	4.06	33 (28%) 1 2	17, 165, 219, 253	2 (1%)
All	All	1297/1461 (88%)	2.48	442 (34%) 1 2	17, 196, 261, 329	2 (0%)

The worst 5 of 442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	783	HIS	47.7
1	A	784	THR	40.3
1	A	729	ASP	37.4
1	A	331	GLU	33.4
4	V	16	GLY	33.1

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 monosaccharides in this entry.

6.4 Ligands ⓘ

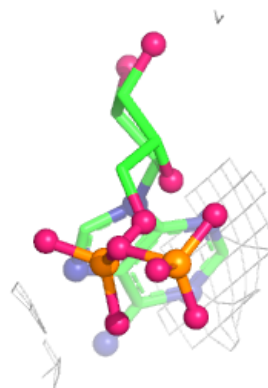
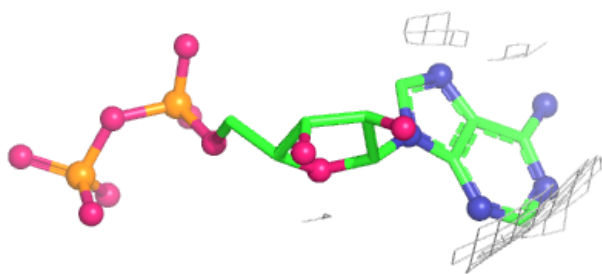
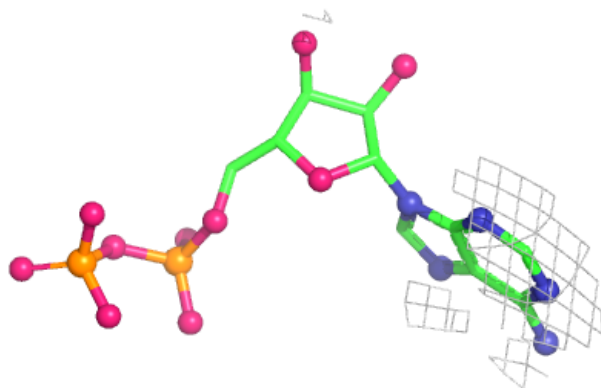
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	1001	1/1	0.55	0.32	156,156,156,156	0
8	TBR	Y	503	18/18	0.62	0.15	222,330,362,376	18
8	TBR	A	1018	18/18	0.64	0.14	249,294,327,336	18
8	TBR	A	1017	18/18	0.65	0.12	239,281,307,310	18
8	TBR	A	1014	18/18	0.66	0.11	256,294,322,323	18
8	TBR	A	1010	18/18	0.70	0.10	320,422,488,488	18
6	BEF	A	1002	4/4	0.71	0.14	248,258,259,292	0
8	TBR	A	1016	18/18	0.74	0.15	205,240,270,278	18
7	ADP	A	1003	27/27	0.76	0.12	217,228,242,264	0
8	TBR	A	1009	18/18	0.78	0.10	315,412,481,486	18
8	TBR	A	1006	18/18	0.79	0.08	261,311,368,380	18
8	TBR	A	1015	18/18	0.83	0.18	150,184,202,207	18
8	TBR	Y	502	18/18	0.84	0.12	214,274,323,365	18
8	TBR	A	1013	18/18	0.88	0.15	212,254,282,284	18
8	TBR	Y	501	18/18	0.88	0.10	247,285,334,358	18
8	TBR	A	1008	18/18	0.89	0.15	216,259,385,416	18
8	TBR	A	1007	18/18	0.90	0.08	204,235,270,286	18
8	TBR	A	1004	18/18	0.92	0.06	267,292,333,345	0
8	TBR	A	1005	18/18	0.92	0.06	296,311,356,389	18
8	TBR	A	1011	18/18	0.94	0.06	249,291,340,349	18
8	TBR	A	1012	18/18	0.95	0.05	262,342,436,479	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.