WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 21, 2016 – 03:52 PM EDT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

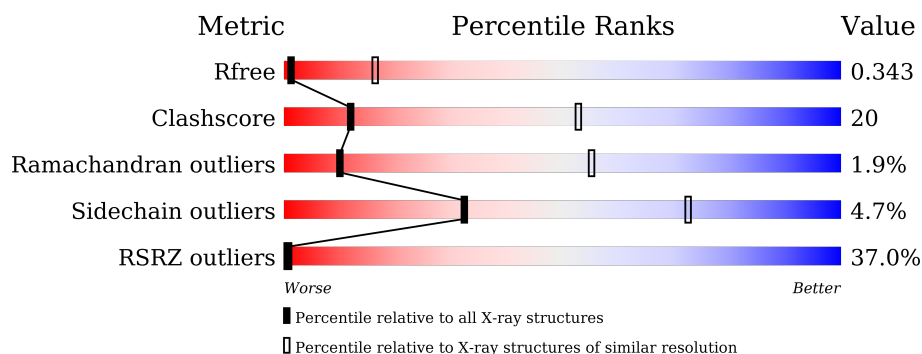|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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	Percentile Ranks	Value
Rfree		0.343
Clashscore		20
Ramachandran outliers		1.9%
Sidechain outliers		4.7%
RSRZ outliers		37.0%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 <=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	836	36% / 60% 25% ·· 11%
2	Y	424	30% / 49% 35% ·· 10%
3	E	70	29% / 56% 23% · 20%
4	V	131	24% / 54% 29% ·· 12%

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 (i)

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
			Total	C	N	O	S			
1	A	746	5876	3677	1030	1135	34	0	0	0

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
			Total	C	N	O	S			
2	Y	380	2936	1951	478	495	12	0	0	0

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
			Total	C	N	O			
3	E	56	460	306	78	76	0	0	0

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
			Total	C	N	O	S			
4	V	115	883	553	153	171	6	0	0	0

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

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

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).
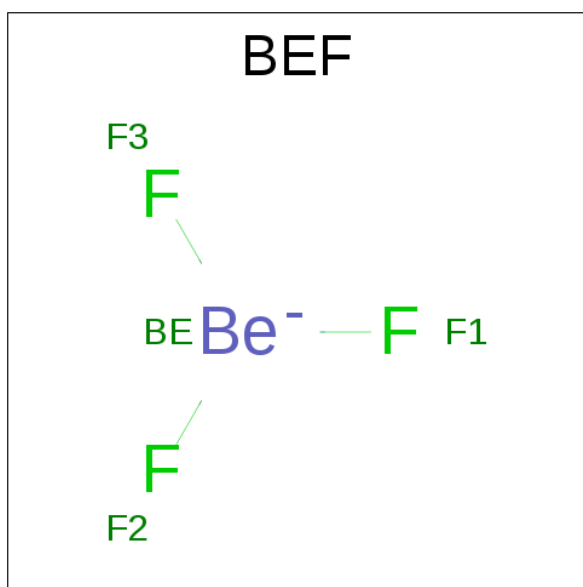
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	Be 1	F 3	0	0

- Molecule 7 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
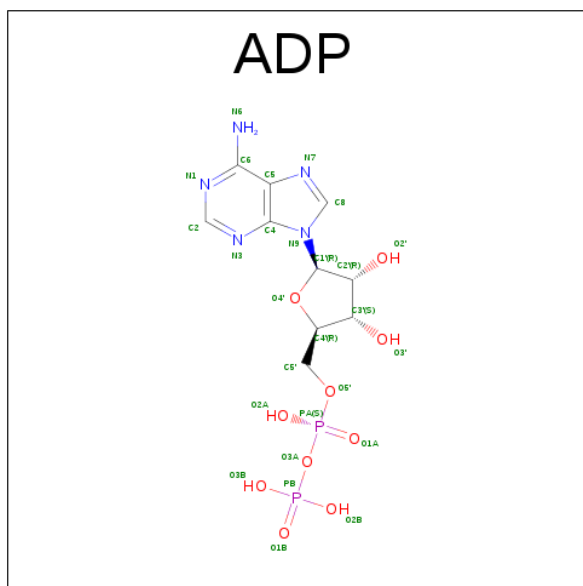
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

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

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

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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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, Insertion Peptide Chimera
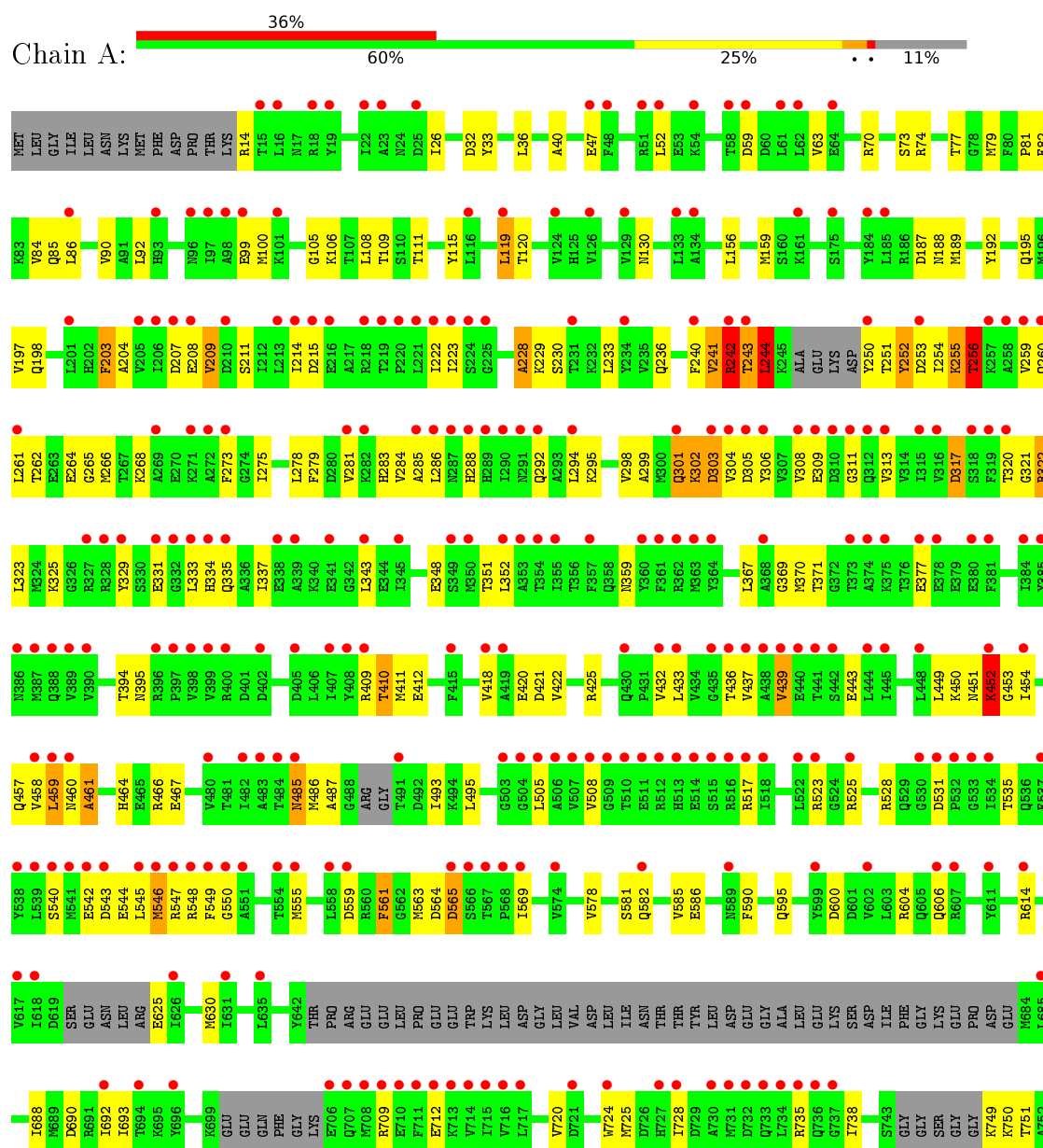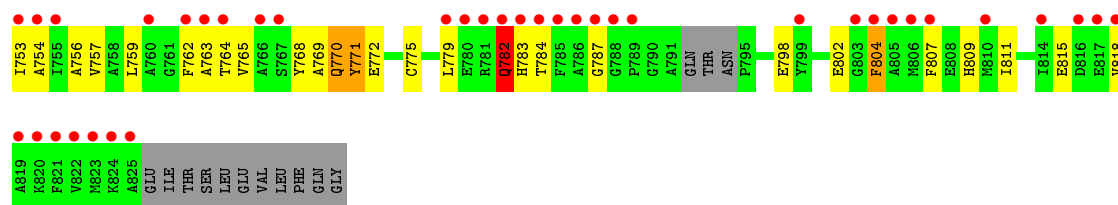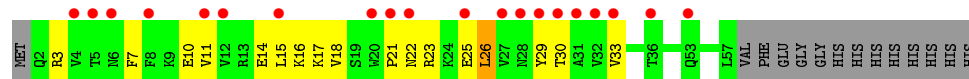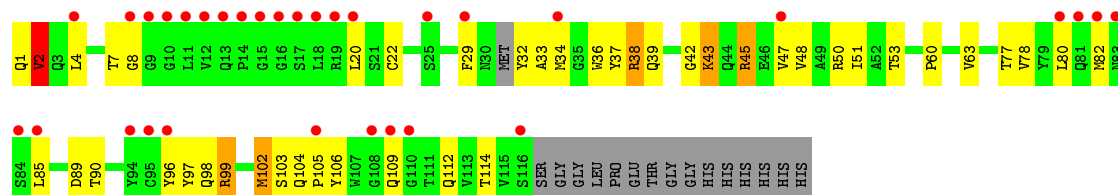
- Molecule 2: Protein translocase subunit SecY

Chain Y:
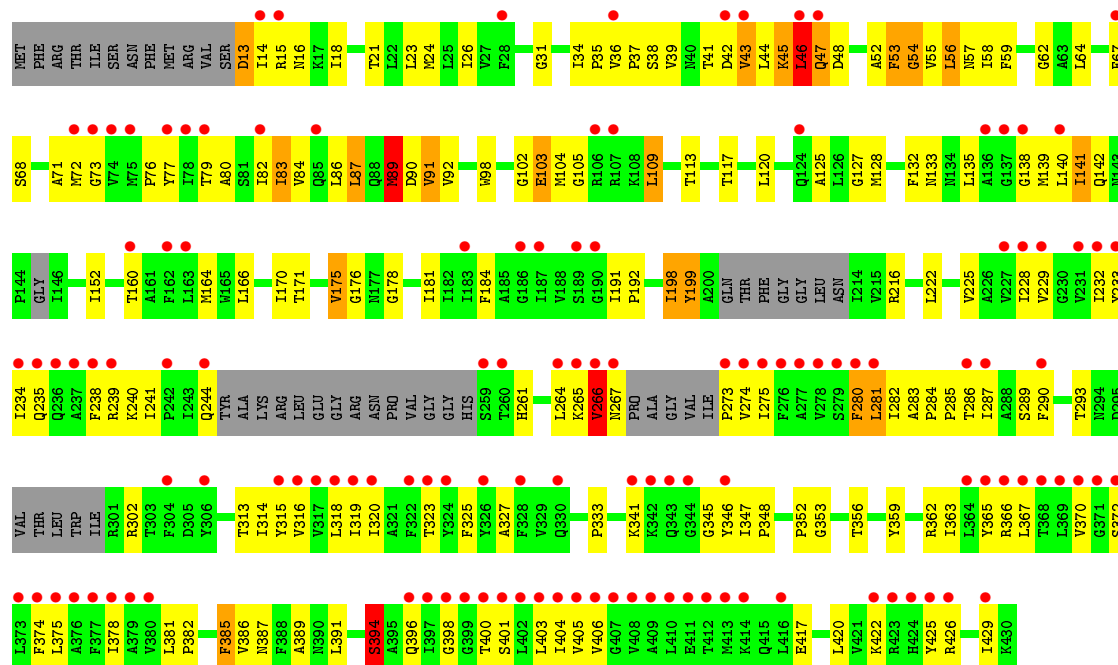
- Molecule 3: Preprotein translocase SecE subunit

Chain E:

- Molecule 4: AYC08

Chain V:

4 Data and refinement statistics (i)

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　–　3.70 110.68　–　3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.85-3.70) 99.9 (110.68-3.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.13 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.295　,　0.315 0.318　,　0.343	Depositor DCC
R_{free} test set	1509 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	191.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 172.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.42, <L^2> = 0.25$	Xtriage
Outliers	3 of 29882 reflections (0.010%)	Xtriage
F_o,F_c correlation	0.67	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, TBR, 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	0.29	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(^{o})	Ideal(^{o})
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 (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	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 (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	730/836 (87%)	676 (93%)	42 (6%)	12 (2%)	12	58
2	Y	368/424 (87%)	335 (91%)	24 (6%)	9 (2%)	7	51
3	E	54/70 (77%)	49 (91%)	4 (7%)	1 (2%)	10	55
4	V	111/131 (85%)	99 (89%)	10 (9%)	2 (2%)	11	56
All	All	1263/1461 (86%)	1159 (92%)	80 (6%)	24 (2%)	10	55

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 (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	622/706 (88%)	598 (96%)	24 (4%)	39	76
2	Y	313/354 (88%)	293 (94%)	20 (6%)	22	64
3	E	50/63 (79%)	48 (96%)	2 (4%)	38	76
4	V	93/108 (86%)	88 (95%)	5 (5%)	27	69
All	All	1078/1231 (88%)	1027 (95%)	51 (5%)	32	72

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

Mol	Chain	Res	Type
1	A	771	TYR
2	Y	45	LYS
4	V	38	ARG
2	Y	23	LEU
2	Y	46	LEU

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

Mol	Chain	Res	Type
1	A	613	GLN
1	A	739	HIS
2	Y	169	GLN
1	A	605	GLN
2	Y	308	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 carbohydrates 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	0.00	-	0,3,3	0.00	-
7	ADP	A	1003	1,5,6	24,29,29	0.98	1 (4%)	23,45,45	1.74	1 (4%)
8	TBR	A	1004	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1005	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1006	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1007	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1008	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1009	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1010	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1011	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1012	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1013	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1014	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1015	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1016	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1017	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	A	1018	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	Y	501	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	Y	502	-	0,36,36	0.00	-	0,180,180	0.00	-
8	TBR	Y	503	-	0,36,36	0.00	-	0,180,180	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	BEF	A	1002	7	-	0/0/0/0	0/0/0/0
7	ADP	A	1003	1,5,6	-	0/12/32/32	0/3/3/3
8	TBR	A	1004	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1005	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1006	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1007	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1008	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1009	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1010	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1011	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1012	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1013	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1014	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1015	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1016	-	-	0/0/696/696	0/0/19/19

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	TBR	A	1017	-	-	0/0/696/696	0/0/19/19
8	TBR	A	1018	-	-	0/0/696/696	0/0/19/19
8	TBR	Y	501	-	-	0/0/696/696	0/0/19/19
8	TBR	Y	502	-	-	0/0/696/696	0/0/19/19
8	TBR	Y	503	-	-	0/0/696/696	0/0/19/19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1003	ADP	C5-C4	3.11	1.47	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1003	ADP	N3-C2-N1	-6.57	123.71	128.87

There are no chirality outliers.

There are no torsion outliers.

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
7	A	1003	ADP	1	0
8	A	1004	TBR	1	0
8	A	1005	TBR	1	0
8	A	1006	TBR	2	0
8	A	1007	TBR	2	0
8	A	1008	TBR	1	0
8	A	1009	TBR	1	0
8	A	1010	TBR	3	0
8	A	1011	TBR	1	0
8	A	1012	TBR	2	0
8	A	1013	TBR	2	0
8	A	1014	TBR	5	0
8	A	1015	TBR	3	0
8	A	1016	TBR	1	0
8	A	1017	TBR	2	0
8	A	1018	TBR	1	0
8	Y	502	TBR	2	0

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	A	746/836 (89%)	1.91	301 (40%)	0	1	113, 202, 268, 329	0
2	Y	380/424 (89%)	1.71	127 (33%)	0	1	116, 191, 258, 282	0
3	E	56/70 (80%)	1.38	20 (35%)	0	1	155, 220, 261, 265	0
4	V	115/131 (87%)	1.73	32 (27%)	1	1	117, 166, 219, 253	2 (1%)
All	All	1297/1461 (88%)	1.81	480 (37%)	0	1	113, 196, 261, 329	2 (0%)

The worst 5 of 480 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	783	HIS	22.8
1	A	784	THR	15.4
1	A	823	MET	14.8
2	Y	267	ASN	14.8
2	Y	399	GLY	14.1

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 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(Å^2)	Q<0.9
8	TBR	A	1016	18/18	0.94	0.36	1.38	205,240,270,278	18
8	TBR	A	1010	18/18	0.92	0.26	0.59	320,422,488,488	18
8	TBR	A	1015	18/18	0.95	0.31	-0.24	150,184,202,207	18
7	ADP	A	1003	27/27	0.86	0.21	-0.37	217,228,242,264	0
8	TBR	A	1012	18/18	0.99	0.27	-0.46	262,342,436,479	0
8	TBR	A	1004	18/18	0.99	0.27	-0.51	267,292,333,345	0
8	TBR	A	1017	18/18	0.74	0.28	-0.67	239,281,307,310	18
6	BEF	A	1002	4/4	0.88	0.15	-0.75	248,258,259,292	0
8	TBR	A	1009	18/18	0.98	0.18	-0.82	315,412,481,486	18
8	TBR	Y	501	18/18	0.97	0.32	-0.89	247,285,334,358	18
8	TBR	A	1007	18/18	0.97	0.29	-0.96	204,235,270,286	18
8	TBR	A	1005	18/18	0.99	0.28	-1.03	296,311,356,389	18
8	TBR	Y	502	18/18	0.97	0.33	-1.05	214,274,323,365	18
8	TBR	A	1011	18/18	0.99	0.27	-1.19	249,291,340,349	18
8	TBR	A	1006	18/18	0.96	0.19	-1.40	261,311,368,380	18
8	TBR	A	1014	18/18	0.94	0.22	-1.54	256,294,322,323	18
8	TBR	A	1013	18/18	0.95	0.21	-1.98	212,254,282,284	18
8	TBR	Y	503	18/18	0.89	0.45	-	222,330,362,376	18
5	MG	A	1001	1/1	0.93	0.27	-	156,156,156,156	0
8	TBR	A	1018	18/18	0.87	0.42	-	249,294,327,336	18
8	TBR	A	1008	18/18	0.94	0.39	-	216,259,385,416	18

6.5 Other polymers (i)

There are no such residues in this entry.