



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 10:52 AM EDT

PDB ID : 3UJZ
Title : Crystal structure of enterohemorrhagic E. coli StcE
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Deposited on : 2011-11-08
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

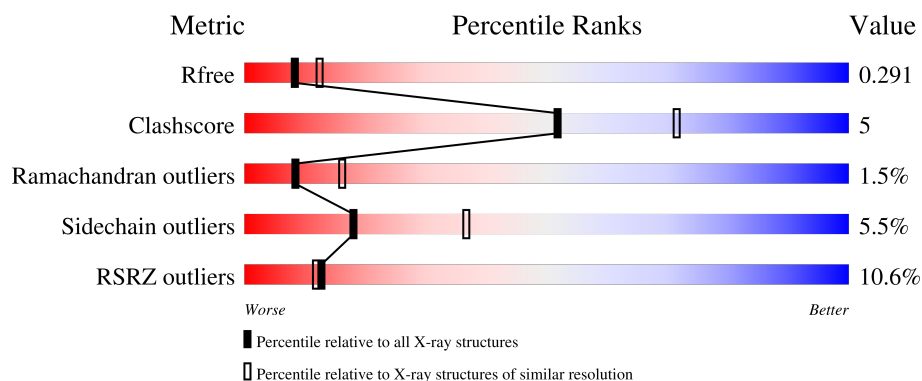
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 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	A	869	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4868 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 Metalloprotease stcE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	Se	0	0	0
			4695	2962	817	900	4	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP O82882
A	31	SER	-	expression tag	UNP O82882
A	32	HIS	-	expression tag	UNP O82882
A	33	MSE	-	expression tag	UNP O82882
A	34	ALA	-	expression tag	UNP O82882
A	35	SER	-	expression tag	UNP O82882
A	318	ALA	LYS	engineered mutation	UNP O82882
A	320	ALA	LYS	engineered mutation	UNP O82882
A	321	ALA	GLU	engineered mutation	UNP O82882
A	447	ASP	GLU	engineered mutation	UNP O82882

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total	O	0	0
			172	172		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.53Å 186.00Å 188.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.50 48.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.17-2.50) 100.0 (48.17-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.211 , 0.253 0.247 , 0.291	Depositor DCC
R_{free} test set	2349 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.954	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4868	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: 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	A	0.51	0/4806	0.72	1/6512 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	881	ASN	N-CA-C	-5.41	96.40	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4695	0	4503	46	0
2	A	1	0	0	0	0
3	A	172	0	0	0	0
All	All	4868	0	4503	46	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 5.

All (46) 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:809:ILE:HG12	1:A:893:MSE:HE1	1.31	1.07
1:A:357:THR:O	1:A:358:ASP:HB2	1.60	1.01
1:A:83:THR:HG22	1:A:542:GLN:HE21	1.34	0.93
1:A:83:THR:HG22	1:A:542:GLN:NE2	1.97	0.79
1:A:300:HIS:HD1	1:A:338:ASN:HD22	1.29	0.76
1:A:516:ASP:OD2	1:A:518:MSE:N	2.22	0.72
1:A:349:MSE:HE1	1:A:353:GLY:HA2	1.70	0.72
1:A:897:TYR:O	1:A:898:LYS:HB2	1.91	0.69
1:A:700:THR:HA	1:A:701:LEU:HB3	1.74	0.68
1:A:105:VAL:HG22	1:A:277:ILE:HG12	1.78	0.65
1:A:130:ILE:HG12	1:A:527:ALA:HB1	1.79	0.64
1:A:822:VAL:HG11	1:A:897:TYR:CD2	2.35	0.62
1:A:93:ARG:HB2	1:A:259:ILE:HG12	1.81	0.62
1:A:357:THR:O	1:A:358:ASP:CB	2.40	0.61
1:A:334:ARG:HD3	1:A:798:GLN:O	2.02	0.60
1:A:501:ASN:O	1:A:502:ASN:HB2	2.03	0.59
1:A:347:GLU:HB3	1:A:355:LEU:HD11	1.84	0.58
1:A:64:ALA:HB3	1:A:89:LEU:HB3	1.85	0.57
1:A:130:ILE:HD11	1:A:482:LYS:HD3	1.88	0.55
1:A:809:ILE:CG1	1:A:893:MSE:HE1	2.22	0.53
1:A:296:GLU:HB2	1:A:550:VAL:HG22	1.91	0.52
1:A:56:SER:HB3	1:A:283:SER:H	1.76	0.51
1:A:881:ASN:O	1:A:883:GLN:N	2.41	0.51
1:A:372:ARG:NH2	1:A:428:SER:OG	2.45	0.50
1:A:765:SER:O	1:A:766:GLN:HB2	2.11	0.50
1:A:822:VAL:CG1	1:A:897:TYR:CD2	2.96	0.49
1:A:366:TRP:O	1:A:372:ARG:NH1	2.46	0.48
1:A:40:SER:HA	1:A:252:ARG:HD2	1.95	0.47
1:A:828:TYR:CE2	1:A:855:ASP:HB3	2.51	0.46
1:A:293:ALA:HB2	1:A:562:TRP:CG	2.53	0.44
1:A:517:ALA:HB2	1:A:531:THR:HB	2.00	0.44
1:A:897:TYR:O	1:A:898:LYS:CB	2.60	0.44
1:A:685:GLY:HA3	1:A:713:TYR:CE1	2.53	0.44
1:A:517:ALA:HB2	1:A:531:THR:CG2	2.48	0.43
1:A:68:ILE:HD12	1:A:476:TRP:HB2	2.01	0.42
1:A:121:TYR:HB3	1:A:125:SER:HB2	2.02	0.42
1:A:300:HIS:NE2	1:A:408:GLN:NE2	2.67	0.42
1:A:45:ASN:HB3	1:A:256:ALA:HB2	2.01	0.42
1:A:501:ASN:O	1:A:502:ASN:CB	2.68	0.41
1:A:414:SER:HB3	1:A:425:HIS:HD2	1.85	0.41
1:A:336:ILE:HD11	1:A:800:LEU:HD21	2.02	0.41
1:A:306:MSE:O	1:A:416:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:SER:O	1:A:754:MSE:SE	2.89	0.40
1:A:311:ARG:HH11	1:A:424:VAL:HG11	1.87	0.40
1:A:475:THR:HG23	1:A:532:MSE:CE	2.52	0.40
1:A:822:VAL:HG11	1:A:897:TYR:CE2	2.56	0.40

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	594/869 (68%)	560 (94%)	25 (4%)	9 (2%)	8	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	789	GLU
1	A	882	GLY
1	A	41	ALA
1	A	358	ASP
1	A	702	SER
1	A	790	GLY
1	A	766	GLN
1	A	856	ASN
1	A	502	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	A	506/716 (71%)	478 (94%)	28 (6%)	18	37

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	84	SER
1	A	110	ASP
1	A	112	ASN
1	A	114	ILE
1	A	130	ILE
1	A	134	ASP
1	A	263	GLU
1	A	308	THR
1	A	313	ARG
1	A	314	PHE
1	A	324	ARG
1	A	354	GLU
1	A	357	THR
1	A	366	TRP
1	A	404	TYR
1	A	414	SER
1	A	422	ILE
1	A	467	ARG
1	A	550	VAL
1	A	692	VAL
1	A	701	LEU
1	A	758	HIS
1	A	789	GLU
1	A	832	ASP
1	A	851	LEU
1	A	881	ASN
1	A	894	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	HIS
1	A	408	GLN
1	A	423	GLN

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Mol	Chain	Res	Type
1	A	528	ASN
1	A	536	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

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	592/869 (68%)	0.78	63 (10%)	13 12	24, 83, 120, 167	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	LEU	9.6
1	A	779	LEU	7.7
1	A	249	GLU	6.8
1	A	767	PRO	6.5
1	A	136	VAL	6.4
1	A	898	LYS	5.9
1	A	697	PRO	5.6
1	A	700	THR	5.6
1	A	514	GLY	5.6
1	A	576	ILE	5.3
1	A	701	LEU	5.3
1	A	358	ASP	4.9
1	A	517	ALA	4.9
1	A	137	PRO	4.8
1	A	718	SER	4.6
1	A	135	GLY	4.0
1	A	515	PHE	3.6
1	A	677	GLU	3.3
1	A	575	THR	3.3
1	A	512	LYS	3.2
1	A	783	SER	3.2
1	A	76	GLY	3.1
1	A	414	SER	3.1
1	A	846	LYS	3.1
1	A	679	ARG	3.1
1	A	285	ARG	3.1
1	A	65	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	699	GLY	2.9
1	A	46	THR	2.9
1	A	516	ASP	2.9
1	A	866	VAL	2.9
1	A	695	TYR	2.8
1	A	250	ASN	2.7
1	A	766	GLN	2.7
1	A	40	SER	2.7
1	A	765	SER	2.6
1	A	392	ASN	2.6
1	A	96	LYS	2.5
1	A	133	LEU	2.5
1	A	357	THR	2.5
1	A	698	GLU	2.5
1	A	555	SER	2.5
1	A	39	ASN	2.4
1	A	812	VAL	2.4
1	A	759	ILE	2.4
1	A	368	SER	2.4
1	A	422	ILE	2.4
1	A	352	THR	2.4
1	A	897	TYR	2.3
1	A	813	ASN	2.3
1	A	100	LYS	2.2
1	A	843	SER	2.2
1	A	513	PHE	2.2
1	A	252	ARG	2.2
1	A	346	LYS	2.2
1	A	405	VAL	2.1
1	A	115	LEU	2.1
1	A	391	LEU	2.1
1	A	504	CYS	2.1
1	A	45	ASN	2.1
1	A	466	HIS	2.0
1	A	845	ALA	2.0
1	A	112	ASN	2.0

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 [i](#)

There are no monosaccharides 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
2	ZN	A	1	1/1	0.98	0.03	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.