



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:26 AM UTC

PDB ID : 8W4G / pdb_00008w4g
Title : Crystal structure of EndoSz mutant D234M, from Streptococcus equi subsp. Zooepidemicus Sz105
Authors : Guan, H.H.; Lin, C.C.; Hsieh, Y.C.; Chen, C.J.
Deposited on : 2023-08-24
Resolution : 2.15 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

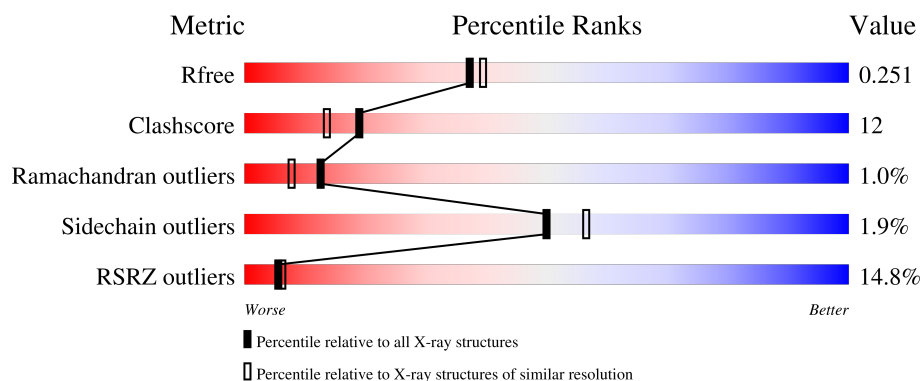
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	992	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7344 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 glycoside hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	876	Total	C	N	O	S	0	0	0
			6902	4375	1152	1360	15			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

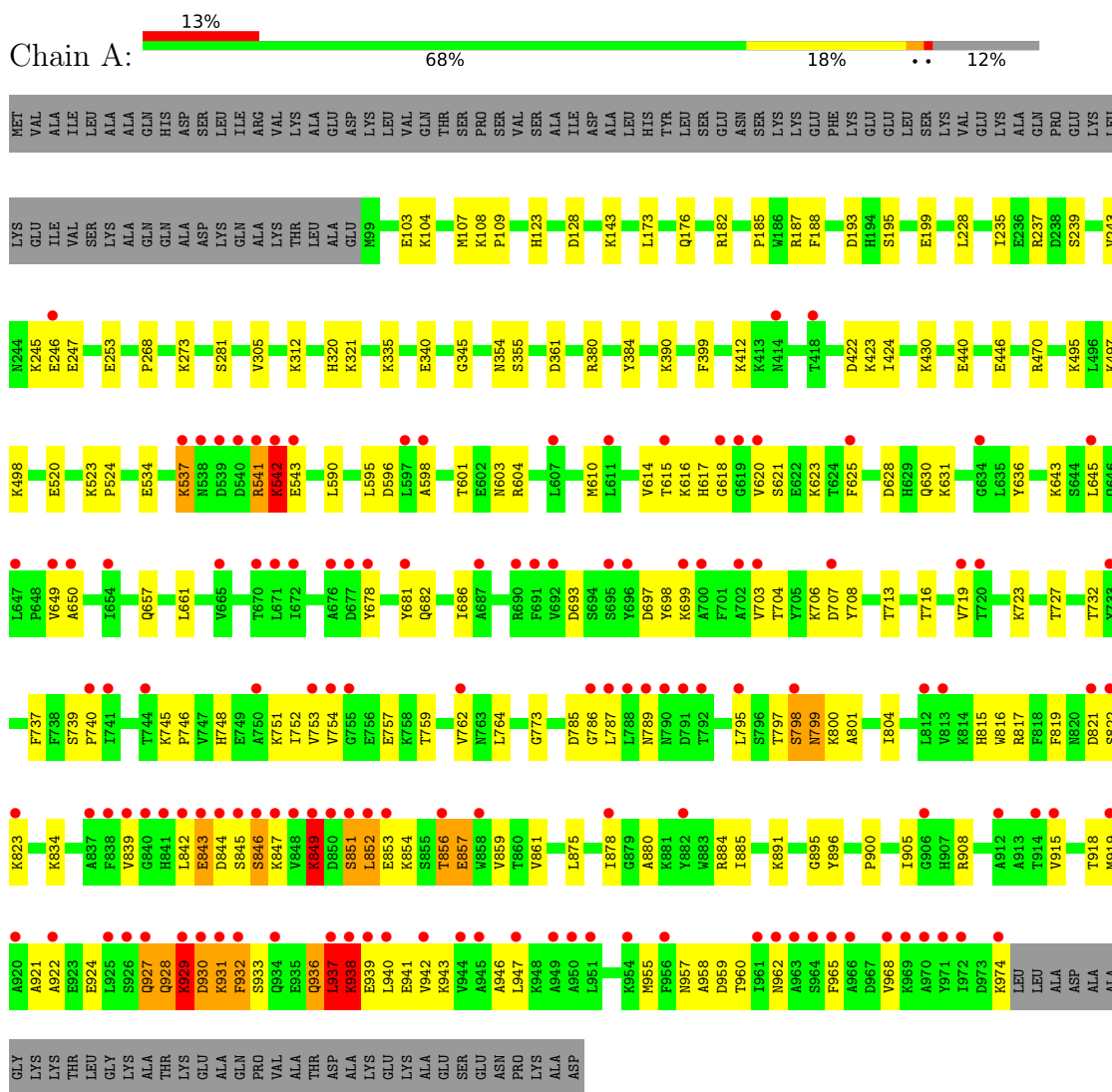
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	441	Total	O	0	0
			441	441		

3 Residue-property plots [i](#)

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 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: glycoside hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.95Å 101.21Å 234.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.57 – 2.15 42.57 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.57-2.15) 99.1 (42.57-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.215 , 0.250 0.218 , 0.251	Depositor DCC
R_{free} test set	3889 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.1	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	0.94	EDS
Total number of atoms	7344	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: CA

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	0.43	0/7035	0.72	14/9501 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	938	LYS	N-CA-C	-10.52	99.81	111.28
1	A	928	GLN	N-CA-C	-10.43	99.91	111.28
1	A	930	ASP	N-CA-C	-8.66	103.78	112.97
1	A	799	ASN	N-CA-C	6.97	125.64	110.80
1	A	937	LEU	N-CA-C	6.84	125.36	110.80
1	A	927	GLN	N-CA-C	-6.20	106.03	113.97
1	A	851	SER	N-CA-C	-6.16	97.67	110.80
1	A	849	LYS	CA-C-N	-6.06	114.25	122.86
1	A	849	LYS	C-N-CA	-6.06	114.25	122.86
1	A	616	LYS	N-CA-C	-5.67	105.25	111.82
1	A	849	LYS	N-CA-C	-5.55	101.64	109.96
1	A	798	SER	CA-C-N	5.37	131.80	121.54
1	A	798	SER	C-N-CA	5.37	131.80	121.54
1	A	928	GLN	CB-CA-C	5.07	119.21	110.79

There are no chirality outliers.

There are no planarity outliers.

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	6902	0	6886	162	0
2	A	1	0	0	0	0
3	A	441	0	0	37	2
All	All	7344	0	6886	162	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 12.

All (162) 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:107:MET:SD	3:A:1495:HOH:O	2.21	0.98
1:A:959:ASP:OD1	3:A:1201:HOH:O	1.87	0.92
1:A:245:LYS:O	3:A:1202:HOH:O	1.94	0.86
1:A:354:ASN:OD1	3:A:1204:HOH:O	1.95	0.85
1:A:534:GLU:OE1	3:A:1203:HOH:O	1.94	0.83
1:A:128:ASP:O	3:A:1205:HOH:O	1.97	0.83
1:A:851:SER:C	1:A:853:GLU:H	1.87	0.81
1:A:253:GLU:OE2	3:A:1206:HOH:O	2.00	0.79
1:A:937:LEU:HB2	1:A:940:LEU:HB3	1.65	0.78
1:A:843:GLU:C	1:A:845:SER:H	1.88	0.78
1:A:108:LYS:HD2	1:A:109:PRO:O	1.84	0.77
1:A:422:ASP:OD2	3:A:1207:HOH:O	2.04	0.76
1:A:603:ASN:OD1	3:A:1209:HOH:O	2.06	0.72
1:A:764:LEU:O	3:A:1208:HOH:O	2.06	0.72
1:A:804:ILE:HD13	1:A:884:ARG:HB2	1.71	0.72
1:A:817:ARG:NH1	3:A:1223:HOH:O	2.23	0.72
1:A:921:ALA:HA	1:A:924:GLU:HG2	1.72	0.72
1:A:937:LEU:HD12	1:A:937:LEU:O	1.90	0.71
1:A:615:THR:HG22	1:A:620:VAL:HG21	1.71	0.71
1:A:716:THR:O	1:A:817:ARG:NH2	2.23	0.71
1:A:247:GLU:OE1	3:A:1210:HOH:O	2.07	0.71
1:A:786:GLY:O	1:A:787:LEU:HD22	1.91	0.70
1:A:706:LYS:N	3:A:1229:HOH:O	2.27	0.68
1:A:412:LYS:O	3:A:1211:HOH:O	2.11	0.68
1:A:851:SER:C	1:A:853:GLU:N	2.51	0.67
1:A:852:LEU:HB2	1:A:854:LYS:HE3	1.77	0.67
1:A:843:GLU:C	1:A:845:SER:N	2.49	0.67
1:A:104:LYS:HD2	3:A:1495:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLU:OE2	3:A:1212:HOH:O	2.12	0.66
1:A:839:VAL:O	3:A:1213:HOH:O	2.13	0.66
1:A:851:SER:O	1:A:853:GLU:N	2.23	0.66
1:A:603:ASN:ND2	3:A:1227:HOH:O	2.26	0.65
1:A:941:GLU:C	1:A:943:LYS:H	2.05	0.65
1:A:800:LYS:NZ	3:A:1234:HOH:O	2.29	0.65
1:A:143:LYS:NZ	3:A:1233:HOH:O	2.29	0.65
1:A:798:SER:O	3:A:1214:HOH:O	2.14	0.64
1:A:924:GLU:HA	1:A:927:GLN:HB2	1.78	0.63
1:A:237:ARG:NH1	3:A:1228:HOH:O	2.26	0.63
1:A:542:LYS:HA	1:A:542:LYS:NZ	2.14	0.62
1:A:928:GLN:HG2	1:A:930:ASP:OD1	1.99	0.62
1:A:933:SER:HA	1:A:936:GLN:HB2	1.82	0.62
1:A:773:GLY:O	3:A:1215:HOH:O	2.16	0.61
1:A:797:THR:HG21	1:A:800:LYS:O	2.01	0.60
1:A:931:LYS:O	1:A:931:LYS:NZ	2.22	0.60
1:A:918:THR:O	1:A:922:ALA:N	2.35	0.59
1:A:390:LYS:NZ	3:A:1226:HOH:O	2.26	0.59
1:A:822:SER:O	1:A:823:LYS:HB3	2.03	0.58
1:A:957:ASN:ND2	1:A:960:THR:OG1	2.37	0.58
1:A:843:GLU:O	1:A:845:SER:N	2.36	0.58
1:A:195:SER:OG	1:A:199:GLU:HG2	2.04	0.58
1:A:678:TYR:O	1:A:682:GLN:HG3	2.03	0.57
1:A:697:ASP:OD1	1:A:698:TYR:N	2.36	0.57
1:A:320:HIS:O	3:A:1216:HOH:O	2.17	0.57
1:A:759:THR:O	3:A:1217:HOH:O	2.17	0.57
1:A:713:THR:HG23	1:A:719:VAL:HG22	1.87	0.57
1:A:103:GLU:OE2	3:A:1218:HOH:O	2.17	0.57
1:A:123:HIS:HE1	1:A:424:ILE:HD12	1.69	0.57
1:A:819:PHE:O	1:A:900:PRO:HD2	2.05	0.56
1:A:103:GLU:CD	1:A:104:LYS:H	2.15	0.55
1:A:861:VAL:HG12	1:A:875:LEU:HD22	1.88	0.55
1:A:799:ASN:ND2	3:A:1243:HOH:O	2.35	0.55
1:A:520:GLU:OE1	3:A:1219:HOH:O	2.18	0.55
1:A:928:GLN:HG2	1:A:930:ASP:CG	2.32	0.55
1:A:762:VAL:HG21	1:A:908:ARG:HE	1.71	0.55
1:A:498:LYS:NZ	3:A:1253:HOH:O	2.40	0.55
1:A:804:ILE:HD11	1:A:884:ARG:HD3	1.90	0.54
1:A:614:VAL:HG21	1:A:625:PHE:CD2	2.43	0.53
1:A:354:ASN:ND2	1:A:355:SER:O	2.41	0.53
1:A:650:ALA:O	1:A:727:THR:OG1	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ILE:HG22	1:A:880:ALA:H	1.74	0.53
1:A:643:LYS:HG3	1:A:748:HIS:HE1	1.74	0.53
1:A:797:THR:OG1	1:A:798:SER:N	2.40	0.52
1:A:846:SER:HB3	1:A:849:LYS:HB3	1.90	0.52
1:A:707:ASP:HB2	1:A:740:PRO:HG3	1.92	0.52
1:A:596:ASP:OD1	1:A:601:THR:HG21	2.10	0.52
1:A:933:SER:CA	1:A:936:GLN:HB2	2.40	0.52
1:A:645:LEU:HB2	1:A:752:ILE:HD12	1.93	0.51
1:A:941:GLU:C	1:A:943:LYS:N	2.68	0.51
1:A:598:ALA:HB2	1:A:681:TYR:HE1	1.76	0.51
1:A:542:LYS:HA	1:A:542:LYS:HZ1	1.75	0.50
1:A:345:GLY:HA3	1:A:399:PHE:CZ	2.47	0.50
1:A:708:TYR:CZ	1:A:739:SER:HB2	2.46	0.50
1:A:856:THR:OG1	1:A:857:GLU:N	2.45	0.50
1:A:361:ASP:OD1	1:A:380:ARG:HD2	2.12	0.49
1:A:943:LYS:HZ3	1:A:946:ALA:HB3	1.77	0.49
1:A:943:LYS:HG3	1:A:968:VAL:CG2	2.42	0.49
1:A:657:GLN:CB	1:A:723:LYS:HD3	2.42	0.49
1:A:795:LEU:HD21	1:A:896:TYR:C	2.37	0.49
1:A:929:LYS:C	1:A:931:LYS:H	2.19	0.49
1:A:108:LYS:HE2	3:A:1582:HOH:O	2.13	0.48
1:A:928:GLN:CG	1:A:930:ASP:OD1	2.62	0.48
1:A:815:HIS:HB3	1:A:905:ILE:HB	1.96	0.48
1:A:974:LYS:N	1:A:974:LYS:HD2	2.29	0.48
1:A:799:ASN:HB2	1:A:895:GLY:HA3	1.96	0.47
1:A:941:GLU:O	1:A:943:LYS:N	2.46	0.47
1:A:958:ALA:O	1:A:962:ASN:ND2	2.47	0.47
1:A:697:ASP:OD1	1:A:699:LYS:N	2.48	0.47
1:A:797:THR:O	1:A:896:TYR:HA	2.14	0.47
1:A:617:HIS:CG	1:A:618:GLY:H	2.33	0.47
1:A:657:GLN:HB3	1:A:723:LYS:HD3	1.96	0.47
1:A:929:LYS:HB3	1:A:929:LYS:HE2	1.41	0.46
1:A:235:ILE:O	1:A:281:SER:HA	2.16	0.46
1:A:620:VAL:N	3:A:1265:HOH:O	2.48	0.46
1:A:732:THR:HG23	1:A:753:VAL:HG22	1.96	0.46
1:A:919:MET:HG3	1:A:947:LEU:HD22	1.97	0.46
1:A:628:ASP:OD1	1:A:628:ASP:N	2.49	0.46
1:A:631:LYS:HE2	1:A:693:ASP:CG	2.41	0.46
1:A:891:LYS:O	3:A:1220:HOH:O	2.21	0.46
1:A:595:LEU:HD12	1:A:630:GLN:NE2	2.31	0.45
1:A:842:LEU:HD23	1:A:842:LEU:HA	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LYS:HA	1:A:430:LYS:HD2	1.57	0.45
1:A:495:LYS:HE2	1:A:495:LYS:HB3	1.73	0.45
1:A:590:LEU:HD11	1:A:610:MET:HE1	1.99	0.45
1:A:523:LYS:HB2	1:A:524:PRO:HD2	1.99	0.45
1:A:816:TRP:CD1	1:A:875:LEU:HD11	2.52	0.45
1:A:636:TYR:CZ	1:A:703:VAL:HG13	2.52	0.45
1:A:595:LEU:HD12	1:A:630:GLN:HE22	1.81	0.44
1:A:834:LYS:O	1:A:885:ILE:HD12	2.18	0.44
1:A:185:PRO:HG2	1:A:188:PHE:CD1	2.53	0.44
1:A:446:GLU:OE2	1:A:470:ARG:NH1	2.51	0.44
1:A:661:LEU:HD22	1:A:737:PHE:CG	2.53	0.43
1:A:789:ASN:ND2	1:A:821:ASP:OD1	2.52	0.43
1:A:924:GLU:HA	1:A:927:GLN:CB	2.44	0.43
1:A:173:LEU:O	1:A:176:GLN:HG2	2.18	0.43
1:A:795:LEU:HD21	1:A:896:TYR:CA	2.48	0.43
1:A:745:LYS:HA	1:A:746:PRO:HD3	1.90	0.43
1:A:955:MET:HE3	1:A:955:MET:HB3	1.84	0.43
1:A:542:LYS:HB3	1:A:543:GLU:H	1.67	0.43
1:A:182:ARG:HB2	1:A:228:LEU:HD12	1.99	0.43
1:A:497:LYS:HE3	3:A:1219:HOH:O	2.17	0.43
1:A:804:ILE:CD1	1:A:884:ARG:HD3	2.48	0.42
1:A:940:LEU:HD12	1:A:940:LEU:O	2.20	0.42
1:A:312:LYS:NZ	3:A:1272:HOH:O	2.51	0.42
1:A:340:GLU:OE1	3:A:1221:HOH:O	2.22	0.42
1:A:604:ARG:CZ	1:A:686:ILE:HG12	2.49	0.42
1:A:798:SER:O	1:A:799:ASN:HB3	2.19	0.42
1:A:915:VAL:HG22	1:A:965:PHE:CD2	2.55	0.42
1:A:104:LYS:HA	1:A:104:LYS:HD3	1.81	0.42
1:A:541:ARG:HD3	1:A:542:LYS:HD2	2.01	0.42
1:A:932:PHE:HB3	1:A:933:SER:H	1.56	0.42
1:A:335:LYS:NZ	3:A:1276:HOH:O	2.53	0.42
1:A:187:ARG:HG3	1:A:239:SER:O	2.20	0.41
1:A:537:LYS:NZ	1:A:537:LYS:HB2	2.36	0.41
1:A:852:LEU:CB	1:A:854:LYS:HE3	2.47	0.41
1:A:243:VAL:O	1:A:246:GLU:HG2	2.21	0.41
1:A:305:VAL:HG23	1:A:384:TYR:CE2	2.56	0.41
1:A:423:LYS:HA	1:A:423:LYS:HD2	1.89	0.41
1:A:797:THR:HG22	1:A:801:ALA:HB2	2.02	0.41
1:A:704:THR:OG1	1:A:706:LYS:HG3	2.21	0.41
1:A:937:LEU:O	1:A:938:LYS:C	2.59	0.41
1:A:187:ARG:HD2	1:A:193:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:VAL:HG22	1:A:754:VAL:HG12	2.01	0.40
1:A:751:LYS:HE2	1:A:751:LYS:HB3	1.74	0.40
1:A:541:ARG:HB3	1:A:542:LYS:H	1.61	0.40
1:A:621:SER:C	1:A:623:LYS:H	2.29	0.40
1:A:785:ASP:OD1	1:A:786:GLY:N	2.54	0.40
1:A:797:THR:CG2	1:A:801:ALA:HB2	2.51	0.40
1:A:843:GLU:OE2	1:A:856:THR:HA	2.22	0.40
1:A:757:GLU:HG2	1:A:955:MET:SD	2.61	0.40
1:A:268:PRO:O	1:A:273:LYS:HE3	2.22	0.40
1:A:321:LYS:HE2	1:A:321:LYS:HB3	1.91	0.40
1:A:928:GLN:C	1:A:930:ASP:H	2.30	0.40

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)
3:A:1584:HOH:O	3:A:1599:HOH:O[1_655]	1.87	0.33
3:A:1607:HOH:O	3:A:1626:HOH:O[1_455]	2.02	0.18

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	874/992 (88%)	810 (93%)	55 (6%)	9 (1%)	12 8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	844	ASP
1	A	852	LEU
1	A	937	LEU
1	A	942	VAL

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Mol	Chain	Res	Type
1	A	929	LYS
1	A	932	PHE
1	A	936	GLN
1	A	542	LYS
1	A	847	LYS

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	753/847 (89%)	739 (98%)	14 (2%)	50 56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	LYS
1	A	541	ARG
1	A	542	LYS
1	A	843	GLU
1	A	846	SER
1	A	849	LYS
1	A	856	THR
1	A	857	GLU
1	A	859	VAL
1	A	929	LYS
1	A	931	LYS
1	A	937	LEU
1	A	938	LYS
1	A	939	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	HIS
1	A	441	ASN

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Mol	Chain	Res	Type
1	A	538	ASN
1	A	657	GLN
1	A	742	ASN
1	A	957	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 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 [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, 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	876/992 (88%)	0.86	130 (14%) 5 6	24, 54, 110, 202	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	852	LEU	6.3
1	A	925	LEU	6.1
1	A	787	LEU	5.9
1	A	788	LEU	5.5
1	A	972	ILE	5.4
1	A	848	VAL	5.4
1	A	932	PHE	5.4
1	A	961	ILE	5.3
1	A	944	VAL	5.2
1	A	968	VAL	4.9
1	A	965	PHE	4.7
1	A	842	LEU	4.4
1	A	823	LYS	4.4
1	A	851	SER	4.2
1	A	937	LEU	4.1
1	A	845	SER	4.0
1	A	940	LEU	4.0
1	A	942	VAL	4.0
1	A	798	SER	3.9
1	A	843	GLU	3.6
1	A	970	ALA	3.6
1	A	856	THR	3.5
1	A	754	VAL	3.5
1	A	649	VAL	3.4
1	A	744	THR	3.4
1	A	537	LYS	3.4
1	A	938	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	969	LYS	3.4
1	A	947	LEU	3.3
1	A	949	ALA	3.3
1	A	926	SER	3.2
1	A	692	VAL	3.2
1	A	922	ALA	3.1
1	A	841	HIS	3.1
1	A	671	LEU	3.1
1	A	678	TYR	3.1
1	A	844	ASP	3.1
1	A	849	LYS	3.0
1	A	650	ALA	3.0
1	A	654	ILE	3.0
1	A	847	LYS	3.0
1	A	919	MET	3.0
1	A	795	LEU	2.9
1	A	539	ASP	2.9
1	A	618	GLY	2.9
1	A	840	GLY	2.9
1	A	915	VAL	2.9
1	A	929	LYS	2.9
1	A	813	VAL	2.8
1	A	791	ASP	2.8
1	A	963	ALA	2.8
1	A	966	ALA	2.8
1	A	971	TYR	2.8
1	A	792	THR	2.8
1	A	753	VAL	2.8
1	A	974	LYS	2.7
1	A	681	TYR	2.7
1	A	790	ASN	2.7
1	A	878	ILE	2.7
1	A	945	ALA	2.7
1	A	418	THR	2.7
1	A	956	PHE	2.6
1	A	837	ALA	2.6
1	A	950	ALA	2.6
1	A	733	TYR	2.6
1	A	934	GLN	2.6
1	A	951	LEU	2.6
1	A	543	GLU	2.5
1	A	741	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	670	THR	2.5
1	A	853	GLU	2.5
1	A	691	PHE	2.5
1	A	858	TRP	2.5
1	A	927	GLN	2.5
1	A	615	THR	2.5
1	A	846	SER	2.5
1	A	676	ALA	2.5
1	A	939	GLU	2.4
1	A	822	SER	2.4
1	A	740	PRO	2.4
1	A	611	LEU	2.4
1	A	625	PHE	2.4
1	A	850	ASP	2.4
1	A	920	ALA	2.4
1	A	645	LEU	2.4
1	A	538	ASN	2.4
1	A	672	ILE	2.4
1	A	597	LEU	2.4
1	A	665	VAL	2.4
1	A	703	VAL	2.3
1	A	839	VAL	2.3
1	A	786	GLY	2.3
1	A	542	LYS	2.3
1	A	954	LYS	2.3
1	A	598	ALA	2.3
1	A	964	SER	2.2
1	A	755	GLY	2.2
1	A	696	TYR	2.2
1	A	620	VAL	2.2
1	A	540	ASP	2.2
1	A	677	ASP	2.2
1	A	619	GLY	2.2
1	A	647	LEU	2.2
1	A	414	ASN	2.2
1	A	914	THR	2.2
1	A	930	ASP	2.2
1	A	719	VAL	2.1
1	A	702	ALA	2.1
1	A	699	LYS	2.1
1	A	762	VAL	2.1
1	A	750	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	912	ALA	2.1
1	A	695	SER	2.1
1	A	707	ASP	2.1
1	A	720	THR	2.1
1	A	634	GLY	2.1
1	A	931	LYS	2.1
1	A	687	ALA	2.1
1	A	700	ALA	2.1
1	A	246	GLU	2.1
1	A	690	ARG	2.1
1	A	882	TYR	2.1
1	A	906	GLY	2.1
1	A	838	PHE	2.1
1	A	812	LEU	2.0
1	A	789	ASN	2.0
1	A	962	ASN	2.0
1	A	607	LEU	2.0
1	A	821	ASP	2.0
1	A	541	ARG	2.0

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 oligosaccharides in this entry.

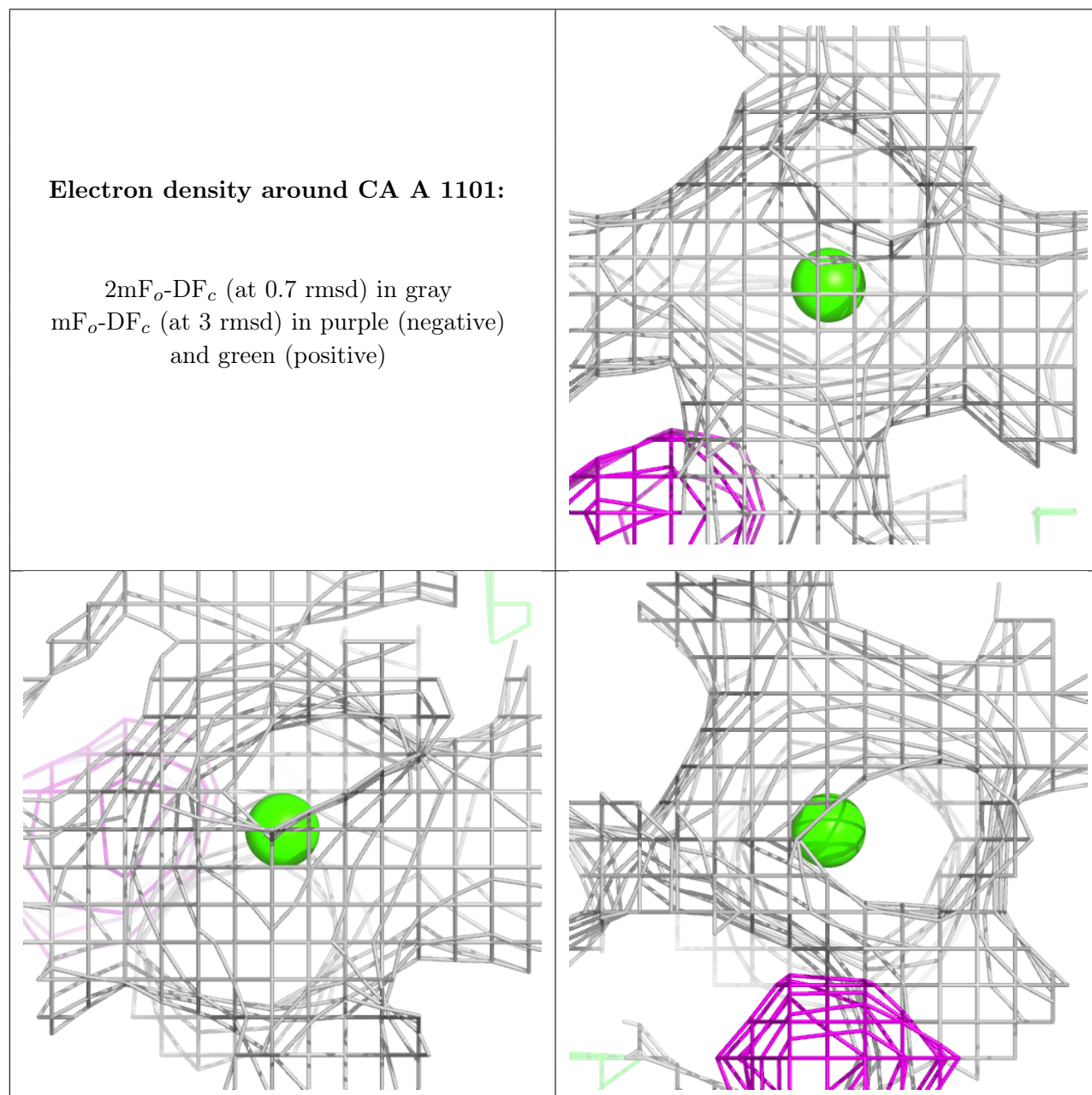
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	CA	A	1101	1/1	0.94	0.11	83,83,83,83	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.