



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 04:49 PM UTC

PDB ID : 8URO / pdb_00008uro
Title : Crystal structure of IgG1-Fc fragment (E382S) in complex with Corynebacterial ENGase CU43 (D187A-E189A)
Authors : Sastre, D.E.; Sultana, N.; Sundberg, E.J.
Deposited on : 2023-10-26
Resolution : 3.62 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

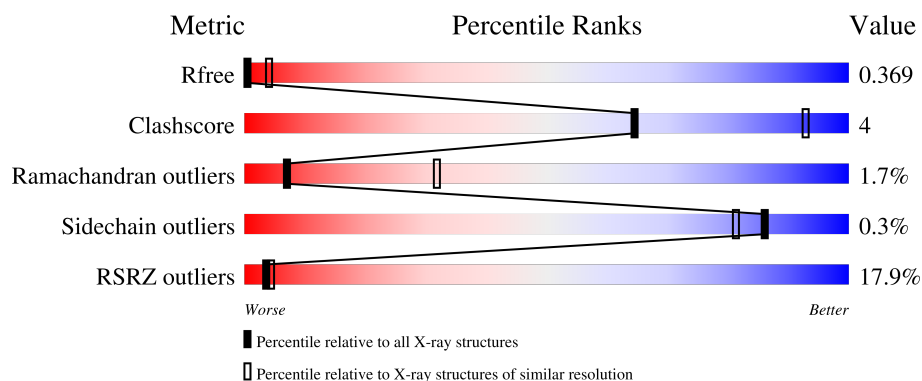
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	415	
1	D	415	
2	B	232	
2	C	232	
2	E	232	

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Mol	Chain	Length	Quality of chain
2	F	232	34% 64% 2% 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9190 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 Corynebacterial protease CP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2328	1460	405	456	7			
1	D	332	Total	C	N	O	S	0	0	0
			2399	1506	418	469	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP A0A830QWM5
A	-1	GLY	-	expression tag	UNP A0A830QWM5
A	0	SER	-	expression tag	UNP A0A830QWM5
A	1	SER	-	expression tag	UNP A0A830QWM5
A	2	HIS	-	expression tag	UNP A0A830QWM5
A	3	HIS	-	expression tag	UNP A0A830QWM5
A	4	HIS	-	expression tag	UNP A0A830QWM5
A	5	HIS	-	expression tag	UNP A0A830QWM5
A	6	HIS	-	expression tag	UNP A0A830QWM5
A	7	HIS	-	expression tag	UNP A0A830QWM5
A	8	SER	-	expression tag	UNP A0A830QWM5
A	9	SER	-	expression tag	UNP A0A830QWM5
A	10	GLY	-	expression tag	UNP A0A830QWM5
A	11	LEU	-	expression tag	UNP A0A830QWM5
A	12	VAL	-	expression tag	UNP A0A830QWM5
A	13	PRO	-	expression tag	UNP A0A830QWM5
A	14	ARG	-	expression tag	UNP A0A830QWM5
A	15	GLY	-	expression tag	UNP A0A830QWM5
A	16	SER	-	expression tag	UNP A0A830QWM5
A	17	HIS	-	expression tag	UNP A0A830QWM5
A	18	MET	-	expression tag	UNP A0A830QWM5
A	19	ALA	-	expression tag	UNP A0A830QWM5
A	20	SER	-	expression tag	UNP A0A830QWM5
A	21	MET	-	expression tag	UNP A0A830QWM5
A	22	THR	-	expression tag	UNP A0A830QWM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP A0A830QWM5
A	24	GLY	-	expression tag	UNP A0A830QWM5
A	25	GLN	-	expression tag	UNP A0A830QWM5
A	26	GLN	-	expression tag	UNP A0A830QWM5
A	27	MET	-	expression tag	UNP A0A830QWM5
A	28	GLY	-	expression tag	UNP A0A830QWM5
A	29	ARG	-	expression tag	UNP A0A830QWM5
A	30	GLY	-	expression tag	UNP A0A830QWM5
A	31	SER	-	expression tag	UNP A0A830QWM5
A	187	ALA	ASP	engineered mutation	UNP A0A830QWM5
A	189	ALA	GLU	engineered mutation	UNP A0A830QWM5
D	-2	MET	-	expression tag	UNP A0A830QWM5
D	-1	GLY	-	expression tag	UNP A0A830QWM5
D	0	SER	-	expression tag	UNP A0A830QWM5
D	1	SER	-	expression tag	UNP A0A830QWM5
D	2	HIS	-	expression tag	UNP A0A830QWM5
D	3	HIS	-	expression tag	UNP A0A830QWM5
D	4	HIS	-	expression tag	UNP A0A830QWM5
D	5	HIS	-	expression tag	UNP A0A830QWM5
D	6	HIS	-	expression tag	UNP A0A830QWM5
D	7	HIS	-	expression tag	UNP A0A830QWM5
D	8	SER	-	expression tag	UNP A0A830QWM5
D	9	SER	-	expression tag	UNP A0A830QWM5
D	10	GLY	-	expression tag	UNP A0A830QWM5
D	11	LEU	-	expression tag	UNP A0A830QWM5
D	12	VAL	-	expression tag	UNP A0A830QWM5
D	13	PRO	-	expression tag	UNP A0A830QWM5
D	14	ARG	-	expression tag	UNP A0A830QWM5
D	15	GLY	-	expression tag	UNP A0A830QWM5
D	16	SER	-	expression tag	UNP A0A830QWM5
D	17	HIS	-	expression tag	UNP A0A830QWM5
D	18	MET	-	expression tag	UNP A0A830QWM5
D	19	ALA	-	expression tag	UNP A0A830QWM5
D	20	SER	-	expression tag	UNP A0A830QWM5
D	21	MET	-	expression tag	UNP A0A830QWM5
D	22	THR	-	expression tag	UNP A0A830QWM5
D	23	GLY	-	expression tag	UNP A0A830QWM5
D	24	GLY	-	expression tag	UNP A0A830QWM5
D	25	GLN	-	expression tag	UNP A0A830QWM5
D	26	GLN	-	expression tag	UNP A0A830QWM5
D	27	MET	-	expression tag	UNP A0A830QWM5
D	28	GLY	-	expression tag	UNP A0A830QWM5

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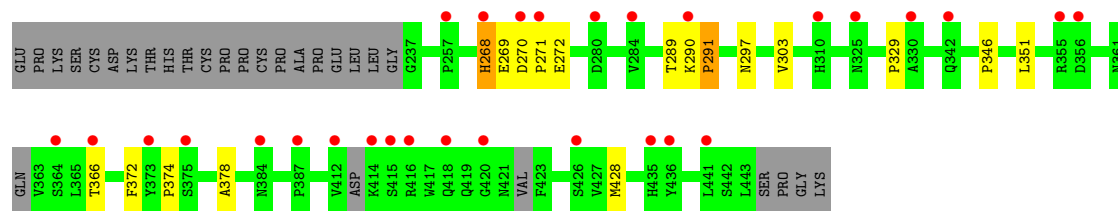
Chain	Residue	Modelled	Actual	Comment	Reference
D	29	ARG	-	expression tag	UNP A0A830QWM5
D	30	GLY	-	expression tag	UNP A0A830QWM5
D	31	SER	-	expression tag	UNP A0A830QWM5
D	187	ALA	ASP	engineered mutation	UNP A0A830QWM5
D	189	ALA	GLU	engineered mutation	UNP A0A830QWM5

- Molecule 2 is a protein called Immunoglobulin gamma-1 heavy chain.

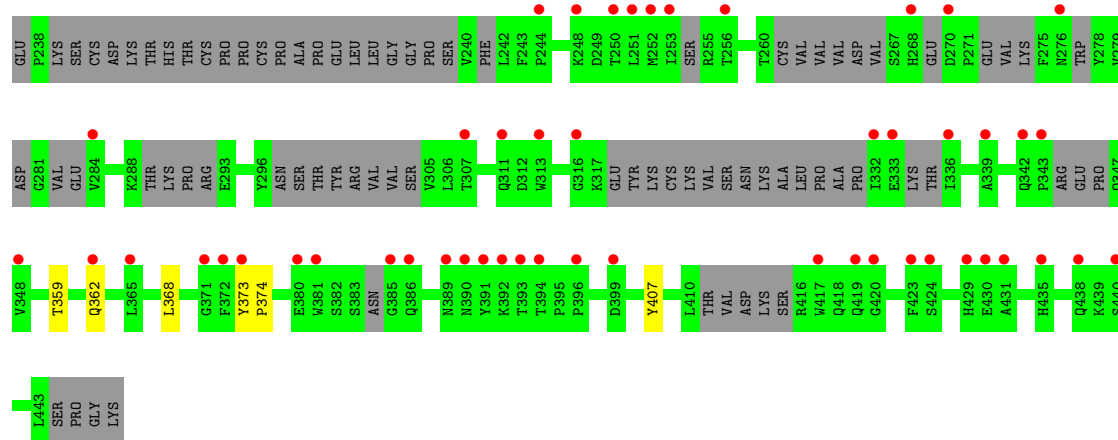
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1401	899	233	263	6			
2	C	152	Total	C	N	O	S	0	0	0
			893	554	162	175	2			
2	E	203	Total	C	N	O	S	0	0	0
			1317	839	228	244	6			
2	F	160	Total	C	N	O	S	0	0	0
			852	512	163	173	4			

There are 4 discrepancies between the modelled and reference sequences:

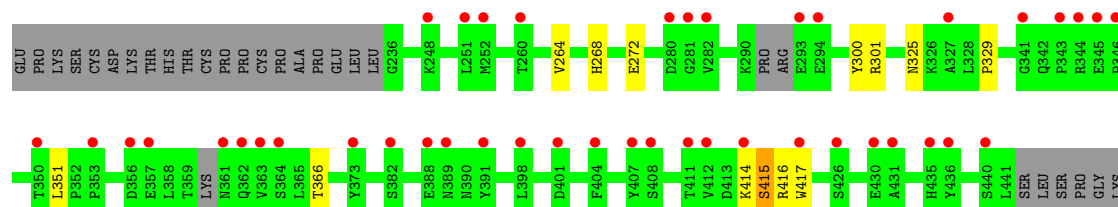
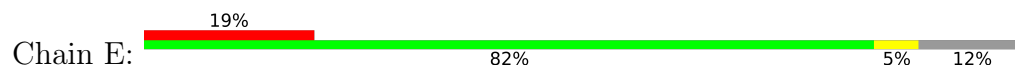
Chain	Residue	Modelled	Actual	Comment	Reference
B	382	SER	GLU	engineered mutation	UNP P0DOX5
C	382	SER	GLU	engineered mutation	UNP P0DOX5
E	382	SER	GLU	engineered mutation	UNP P0DOX5
F	382	SER	GLU	engineered mutation	UNP P0DOX5



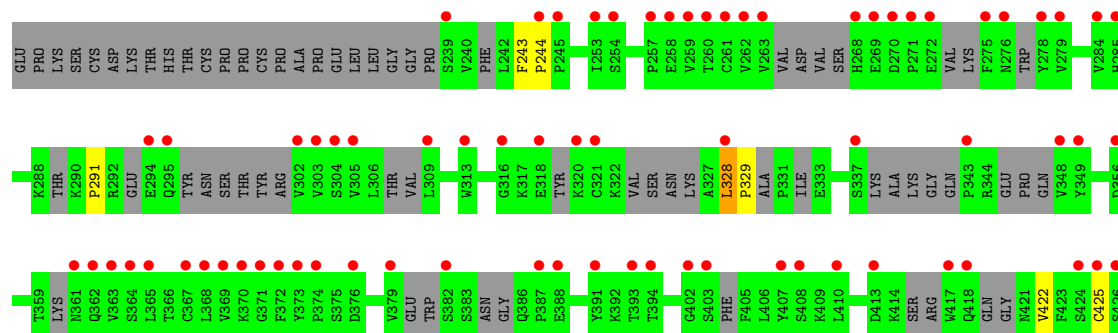
• Molecule 2: Immunoglobulin gamma-1 heavy chain

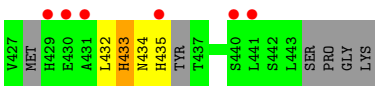


• Molecule 2: Immunoglobulin gamma-1 heavy chain



• Molecule 2: Immunoglobulin gamma-1 heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.44Å 81.99Å 148.10Å 90.00° 113.20° 90.00°	Depositor
Resolution (Å)	33.96 – 3.62 33.96 – 3.62	Depositor EDS
% Data completeness (in resolution range)	95.6 (33.96-3.62) 95.4 (33.96-3.62)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.65Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.334 , 0.369 0.334 , 0.369	Depositor DCC
R_{free} test set	1949 reflections (6.17%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 124.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	9190	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.30% 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

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	0.09	0/2377	0.29	0/3254
1	D	0.09	0/2447	0.28	0/3340
2	B	0.12	0/1438	0.38	0/1985
2	C	0.10	0/897	0.30	0/1227
2	E	0.10	0/1348	0.31	0/1867
2	F	0.14	0/837	0.33	0/1132
All	All	0.10	0/9344	0.31	0/12805

There are no bond length outliers.

There are no bond angle outliers.

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	2328	0	1949	23	0
1	D	2399	0	2099	24	0
2	B	1401	0	1158	8	0
2	C	893	0	567	2	0
2	E	1317	0	1044	7	0
2	F	852	0	430	3	0
All	All	9190	0	7247	64	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 4.

All (64) 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:D:120:PHE:HA	1:D:124:TYR:HB2	1.70	0.73
1:A:120:PHE:HA	1:A:124:TYR:HB2	1.72	0.72
1:D:66:TYR:HB2	1:D:332:TYR:HA	1.76	0.67
1:A:66:TYR:HD2	1:A:332:TYR:HD1	1.41	0.67
1:D:191:ARG:HG2	1:D:244:LEU:HD22	1.79	0.64
1:D:264:LYS:HD2	1:D:269:SER:HB2	1.81	0.63
2:B:351:LEU:HB2	2:B:366:THR:HB	1.83	0.61
2:F:328:LEU:O	2:F:329:PRO:C	2.46	0.59
1:A:68:ARG:HH21	1:A:70:TRP:HE1	1.51	0.56
1:D:144:LEU:O	1:D:148:ILE:HG12	2.06	0.56
2:C:368:LEU:HD13	2:C:407:TYR:CZ	2.41	0.56
1:A:68:ARG:HH21	1:A:70:TRP:NE1	2.05	0.55
2:E:264:VAL:HG12	2:E:301:ARG:HG3	1.88	0.55
2:E:415:SER:O	2:E:417:TRP:N	2.41	0.54
1:D:297:ASP:O	1:D:298:THR:HG22	2.07	0.54
2:B:268:HIS:O	2:B:270:ASP:N	2.31	0.53
1:D:321:PRO:HD3	1:D:326:LYS:HB3	1.90	0.53
2:B:289:THR:C	2:B:291:PRO:HD3	2.34	0.52
1:A:66:TYR:HB2	1:A:332:TYR:HA	1.93	0.50
1:A:227:GLY:N	1:A:233:TYR:OH	2.45	0.49
1:D:137:ARG:HG2	1:D:175:TYR:HD2	1.78	0.49
1:D:227:GLY:N	1:D:233:TYR:OH	2.46	0.49
1:A:321:PRO:HD3	1:A:326:LYS:HB3	1.94	0.49
2:F:432:LEU:O	2:F:434:ASN:N	2.46	0.48
1:D:211:SER:HB3	1:D:253:VAL:HB	1.96	0.48
2:B:346:PRO:HB3	2:B:372:PHE:HB3	1.96	0.47
2:E:272:GLU:O	2:E:325:ASN:ND2	2.41	0.46
2:E:351:LEU:HB2	2:E:366:THR:HB	1.97	0.46
1:A:66:TYR:HD2	1:A:332:TYR:CD1	2.29	0.46
1:D:197:THR:HG23	2:E:329:PRO:HD3	1.97	0.46
2:B:290:LYS:N	2:B:291:PRO:HD3	2.30	0.45
1:A:64:PHE:HE1	1:A:66:TYR:CE1	2.34	0.45
1:A:137:ARG:HG2	1:A:175:TYR:HD2	1.80	0.45
1:A:53:ALA:HA	1:A:283:SER:HB3	1.97	0.45
2:C:373:TYR:HB3	2:C:374:PRO:HD3	1.98	0.45
1:A:157:SER:HA	1:A:201:TRP:CH2	2.53	0.44
1:D:297:ASP:C	1:D:299:ASN:H	2.26	0.44
1:A:314:MET:HE3	1:A:356:PHE:HD1	1.82	0.44
2:B:378:ALA:HB3	2:B:428:MET:HB2	2.00	0.43
1:A:211:SER:HB3	1:A:253:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:HA	1:A:131:ARG:HD3	1.99	0.43
2:E:268:HIS:HA	2:E:300:TYR:HE2	1.83	0.43
1:D:287:LEU:HG	1:D:328:GLY:N	2.34	0.43
1:A:66:TYR:CD2	1:A:332:TYR:HD1	2.30	0.43
1:D:274:TRP:O	1:D:278:ARG:N	2.52	0.43
1:D:193:VAL:O	1:D:200:ARG:HG3	2.18	0.43
1:D:64:PHE:HB3	1:D:330:PHE:CB	2.49	0.42
1:D:314:MET:HE3	1:D:356:PHE:HD1	1.84	0.42
1:A:287:LEU:HG	1:A:328:GLY:N	2.34	0.42
2:B:291:PRO:HG2	2:B:303:VAL:HB	2.00	0.42
2:F:433:HIS:C	2:F:435:HIS:H	2.27	0.42
1:D:200:ARG:HE	2:E:329:PRO:HG2	1.84	0.42
1:A:275:ASN:O	1:A:278:ARG:HG2	2.20	0.42
1:D:53:ALA:HA	1:D:283:SER:HB3	2.00	0.42
1:A:47:GLN:HB2	1:A:51:VAL:HG11	2.02	0.41
1:D:55:ALA:HA	1:D:324:GLY:HA2	2.03	0.41
1:D:191:ARG:HE	1:D:244:LEU:HD13	1.85	0.41
1:D:275:ASN:O	1:D:278:ARG:HG2	2.20	0.41
1:A:203:LEU:HD23	1:A:249:LEU:HD12	2.02	0.41
1:D:256:TYR:HB3	1:D:287:LEU:HD13	2.03	0.41
1:D:64:PHE:CZ	1:D:102:SER:HB3	2.56	0.40
1:A:43:ALA:HB1	2:B:329:PRO:O	2.22	0.40
1:A:100:MET:HG3	1:A:134:LYS:HB2	2.02	0.40
1:A:297:ASP:C	1:A:299:ASN:H	2.28	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	328/415 (79%)	310 (94%)	14 (4%)	4 (1%)	10 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	326/415 (79%)	312 (96%)	14 (4%)	0	100	100
2	B	196/232 (84%)	180 (92%)	9 (5%)	7 (4%)	2	20
2	C	121/232 (52%)	114 (94%)	5 (4%)	2 (2%)	7	32
2	E	197/232 (85%)	192 (98%)	2 (1%)	3 (2%)	8	34
2	F	115/232 (50%)	104 (90%)	5 (4%)	6 (5%)	1	14
All	All	1283/1758 (73%)	1212 (94%)	49 (4%)	22 (2%)	7	32

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	45	PRO
2	B	291	PRO
2	B	297	ASN
2	B	374	PRO
2	F	244	PRO
2	F	291	PRO
2	F	328	LEU
2	F	422	VAL
2	F	433	HIS
1	A	160	ASP
1	A	162	SER
2	B	269	GLU
2	B	271	PRO
2	C	362	GLN
2	E	415	SER
2	B	268	HIS
2	B	272	GLU
2	C	359	THR
2	E	416	ARG
2	E	414	LYS
2	F	243	PHE

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	189/338 (56%)	188 (100%)	1 (0%)	81	78
1	D	211/338 (62%)	211 (100%)	0	100	100
2	B	124/215 (58%)	124 (100%)	0	100	100
2	C	49/215 (23%)	49 (100%)	0	100	100
2	E	102/215 (47%)	102 (100%)	0	100	100
2	F	27/215 (13%)	26 (96%)	1 (4%)	30	52
All	All	702/1536 (46%)	700 (100%)	2 (0%)	86	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
2	F	425	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	246	GLN
1	A	292	HIS

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

There are no ligands in this entry.

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	332/415 (80%)	0.83	28 (8%) 17 13	56, 87, 128, 164	0
1	D	332/415 (80%)	0.76	19 (5%) 29 19	57, 86, 134, 154	0
2	B	204/232 (87%)	1.08	29 (14%) 6 7	59, 98, 147, 171	0
2	C	152/232 (65%)	1.68	50 (32%) 1 1	110, 163, 202, 207	0
2	E	203/232 (87%)	1.41	43 (21%) 2 3	65, 122, 177, 225	0
2	F	160/232 (68%)	2.12	79 (49%) 0 0	89, 170, 194, 208	0
All	All	1383/1758 (78%)	1.18	248 (17%) 3 4	56, 99, 184, 225	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	280	ASP	7.0
1	D	341	TYR	6.2
2	E	294	GLU	5.8
2	F	305	VAL	5.7
2	C	380	GLU	5.4
2	F	260	THR	5.4
2	F	262	VAL	5.2
1	A	341	TYR	5.1
2	F	367	CYS	5.1
2	F	258	GLU	5.1
2	C	420	GLY	4.9
2	F	316	GLY	4.7
2	F	373	TYR	4.6
2	C	429	HIS	4.6
1	A	88	HIS	4.5
2	C	393	THR	4.3
2	E	361	ASN	4.3
2	C	336	ILE	4.2
2	F	278	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
2	E	357	GLU	4.2
2	F	254	SER	4.2
2	F	285	HIS	4.2
2	E	363	VAL	4.1
2	E	293	GLU	4.1
2	F	284	VAL	4.1
2	F	263	VAL	4.1
2	F	245	PRO	4.1
2	E	362	GLN	4.0
2	E	388	GLU	4.0
2	F	424	SER	4.0
1	A	85	ASP	3.9
2	F	407	TYR	3.9
1	D	161	ASP	3.8
2	E	341	GLY	3.8
2	F	313	TRP	3.7
2	F	391	TYR	3.6
2	B	356	ASP	3.6
2	E	407	TYR	3.6
2	C	284	VAL	3.6
2	F	303	VAL	3.6
2	F	429	HIS	3.5
2	C	396	PRO	3.5
1	A	83	TRP	3.5
2	C	424	SER	3.5
2	C	365	LEU	3.4
2	C	435	HIS	3.4
2	E	401	ASP	3.4
2	F	279	VAL	3.4
2	F	393	THR	3.3
1	D	182	ASP	3.3
2	F	270	ASP	3.3
2	F	343	PRO	3.3
2	F	261	CYS	3.3
1	A	51	VAL	3.2
2	F	348	VAL	3.2
2	F	418	GLN	3.2
2	C	339	ALA	3.2
2	F	244	PRO	3.2
2	C	276	ASN	3.2
2	B	415	SER	3.2
2	B	373	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	268	HIS	3.1
1	A	59	ALA	3.1
1	D	79	ASP	3.1
2	E	251	LEU	3.1
2	E	350	THR	3.1
2	F	269	GLU	3.1
2	C	419	GLN	3.1
1	A	44	SER	3.1
2	E	356	ASP	3.1
2	F	239	SER	3.0
2	E	431	ALA	3.0
2	F	430	GLU	3.0
2	C	332	ILE	3.0
1	A	324	GLY	3.0
1	A	39	ALA	3.0
2	B	271	PRO	3.0
2	E	344	ARG	2.9
1	A	182	ASP	2.9
2	E	343	PRO	2.9
2	B	418	GLN	2.9
2	B	414	LYS	2.9
2	C	268	HIS	2.9
2	F	394	THR	2.9
1	D	83	TRP	2.9
2	C	381	TRP	2.9
1	D	304	ALA	2.9
1	A	237	ASP	2.8
2	C	391	TYR	2.8
2	B	364	SER	2.8
2	F	441	LEU	2.8
2	E	408	SER	2.8
2	C	438	GLN	2.8
2	B	270	ASP	2.8
2	F	376	ASP	2.8
2	F	321	CYS	2.8
2	C	392	LYS	2.8
2	F	364	SER	2.7
2	F	403	SER	2.7
2	F	408	SER	2.7
1	D	166	GLU	2.7
2	C	372	PHE	2.7
2	F	410	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	259	VAL	2.7
2	E	346	PRO	2.7
1	A	150	GLU	2.7
2	F	318	GLU	2.6
2	E	260	THR	2.6
2	F	425	CYS	2.6
2	C	385	GLY	2.6
2	E	281	GLY	2.6
2	F	257	PRO	2.6
2	E	404	PHE	2.6
1	A	160	ASP	2.6
2	C	371	GLY	2.6
2	B	426	SER	2.5
2	E	248	LYS	2.5
2	F	272	GLU	2.5
2	F	362	GLN	2.5
1	A	81	ASP	2.5
2	F	320	LYS	2.5
2	E	426	SER	2.5
1	A	296	ASN	2.4
2	E	389	ASN	2.4
2	E	411	THR	2.4
2	F	440	SER	2.4
1	D	73	LYS	2.4
2	C	440	SER	2.4
2	C	251	LEU	2.4
2	C	311	GLN	2.4
2	C	386	GLN	2.4
2	C	417	TRP	2.4
2	F	361	ASN	2.4
2	E	364	SER	2.4
2	E	391	TYR	2.4
2	B	310	HIS	2.4
2	F	365	LEU	2.4
2	C	373	TYR	2.4
1	A	305	ILE	2.3
2	B	290	LYS	2.3
2	B	342	GLN	2.3
2	C	342	GLN	2.3
2	C	430	GLU	2.3
2	B	435	HIS	2.3
2	C	394	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	412	VAL	2.3
1	D	39	ALA	2.3
1	A	297	ASP	2.3
2	C	423	PHE	2.3
2	C	343	PRO	2.3
2	F	402	GLY	2.3
2	B	384	ASN	2.3
2	E	436	TYR	2.3
2	F	431	ALA	2.3
2	C	244	PRO	2.3
2	F	374	PRO	2.3
2	C	313	TRP	2.3
2	F	372	PHE	2.3
1	A	300	ARG	2.3
1	D	346	LEU	2.3
2	F	295	GLN	2.3
2	E	382	SER	2.3
2	F	388	GLU	2.3
1	A	265	GLY	2.3
2	B	257	PRO	2.3
2	B	420	GLY	2.3
2	B	416	ARG	2.3
2	F	276	ASN	2.2
2	F	349	TYR	2.2
2	C	248	LYS	2.2
1	A	152	GLY	2.2
2	F	379	VAL	2.2
1	D	41	LEU	2.2
2	C	250	THR	2.2
2	B	355	ARG	2.2
1	A	77	LEU	2.2
2	F	426	SER	2.2
1	D	265	GLY	2.2
2	B	387	PRO	2.2
2	F	271	PRO	2.2
2	F	387	PRO	2.2
1	A	347	THR	2.2
1	D	81	ASP	2.2
1	A	66	TYR	2.2
1	A	250	VAL	2.2
2	B	268	HIS	2.2
2	F	356	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	252	MET	2.2
2	E	252	MET	2.2
2	F	435	HIS	2.2
1	A	70	TRP	2.2
2	C	362	GLN	2.2
2	F	382	SER	2.2
2	E	282	VAL	2.2
2	F	253	ILE	2.2
1	D	325	GLU	2.2
2	E	345	GLU	2.2
2	F	294	GLU	2.2
2	F	371	GLY	2.2
2	C	389	ASN	2.2
2	F	309	LEU	2.2
2	F	413	ASP	2.1
2	F	417	TRP	2.1
2	E	373	TYR	2.1
2	F	302	VAL	2.1
2	E	414	LYS	2.1
2	E	430	GLU	2.1
2	B	325	ASN	2.1
1	A	367	ILE	2.1
2	C	253	ILE	2.1
2	F	275	PHE	2.1
1	D	306	GLY	2.1
2	B	366	THR	2.1
1	A	55	ALA	2.1
1	D	164	TYR	2.1
2	F	328	LEU	2.1
2	C	256	THR	2.1
2	F	304	SER	2.1
1	D	117	TRP	2.1
2	B	436	TYR	2.1
2	E	398	LEU	2.1
2	B	330	ALA	2.1
2	C	431	ALA	2.1
2	C	390	ASN	2.1
2	C	316	GLY	2.1
2	E	353	PRO	2.1
2	E	417	TRP	2.1
2	E	440	SER	2.1
2	F	337	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	284	VAL	2.1
2	C	348	VAL	2.1
2	E	435	HIS	2.0
2	C	270	ASP	2.0
1	D	367	ILE	2.0
2	B	375	SER	2.0
2	E	327	ALA	2.0
2	B	441	LEU	2.0
1	A	348	THR	2.0
2	C	307	THR	2.0
2	C	333	GLU	2.0
2	B	412	VAL	2.0
2	F	369	VAL	2.0
2	F	370	LYS	2.0
1	D	192	GLU	2.0
2	B	280	ASP	2.0
2	C	399	ASP	2.0
2	F	368	LEU	2.0
2	F	363	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.