



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:28 AM UTC

PDB ID : 6QKI / pdb_00006qki
Title : Native structure of EgtB from Chloracidobacterium thermophilum, a type II sulfoxide synthase
Authors : Stampfli, A.R.; Badri, B.N.; Schirmer, T.; Seebeck, F.P.
Deposited on : 2019-01-29
Resolution : 2.04 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

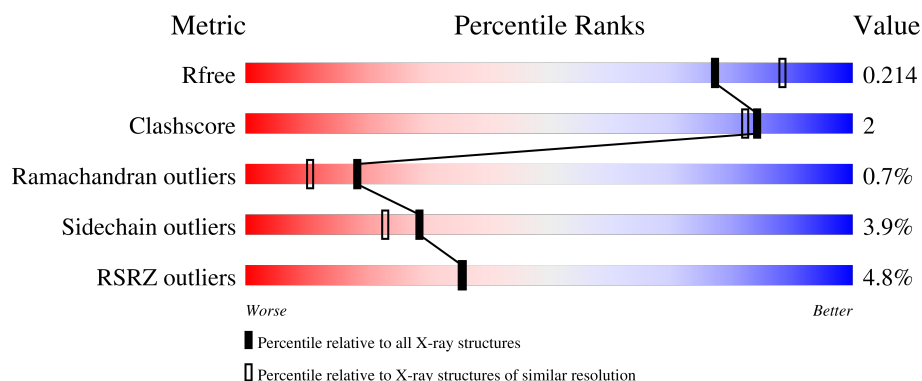
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	437	3% 78% 11% 10%
1	B	437	5% 77% 11% 10%
1	C	437	5% 79% 8% 10%
1	D	437	4% 78% 10% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12935 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	7	0	0
			3193	2049	573	561	10			
1	B	392	Total	C	N	O	S	7	0	0
			3170	2037	569	554	10			
1	C	393	Total	C	N	O	S	0	0	0
			3180	2042	571	557	10			
1	D	392	Total	C	N	O	S	6	0	0
			3167	2034	569	554	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G2LET6
A	-1	SER	-	expression tag	UNP G2LET6
A	0	HIS	-	expression tag	UNP G2LET6
B	-2	GLY	-	expression tag	UNP G2LET6
B	-1	SER	-	expression tag	UNP G2LET6
B	0	HIS	-	expression tag	UNP G2LET6
C	-2	GLY	-	expression tag	UNP G2LET6
C	-1	SER	-	expression tag	UNP G2LET6
C	0	HIS	-	expression tag	UNP G2LET6
D	-2	GLY	-	expression tag	UNP G2LET6
D	-1	SER	-	expression tag	UNP G2LET6
D	0	HIS	-	expression tag	UNP G2LET6

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0

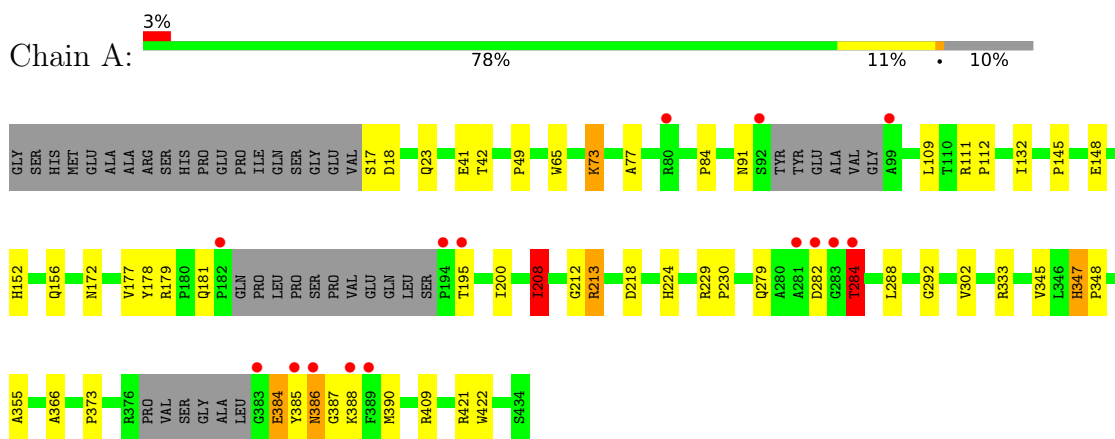
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total 101	O 101	0	0
3	B	65	Total 65	O 65	0	0
3	C	28	Total 28	O 28	0	0
3	D	27	Total 27	O 27	0	0

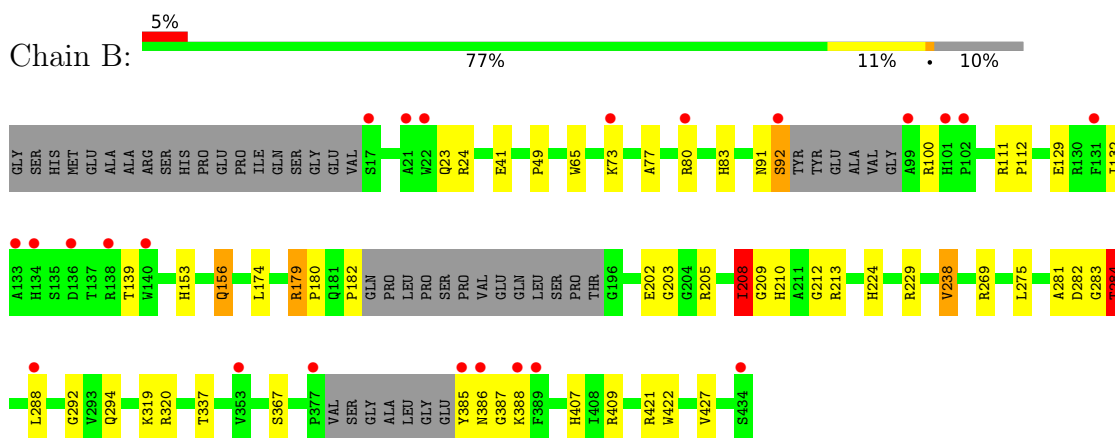
3 Residue-property plots [i](#)

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.

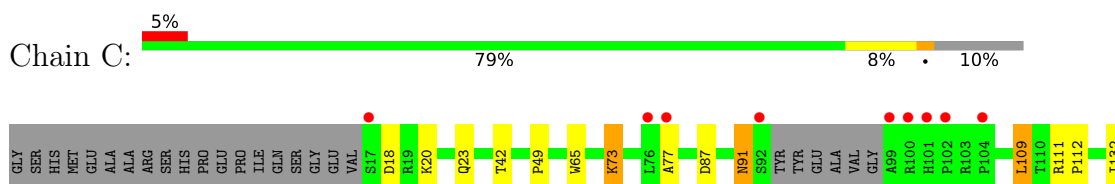
- Molecule 1: Uncharacterized protein

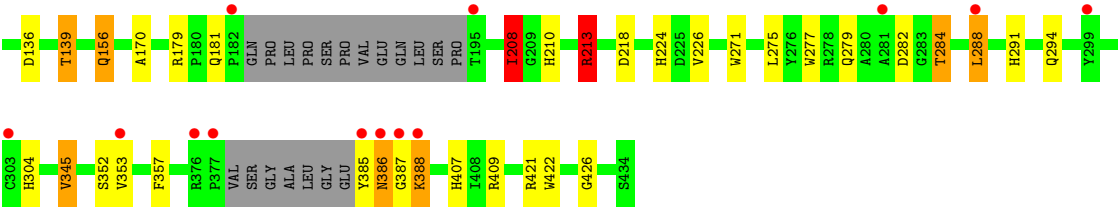


- Molecule 1: Uncharacterized protein

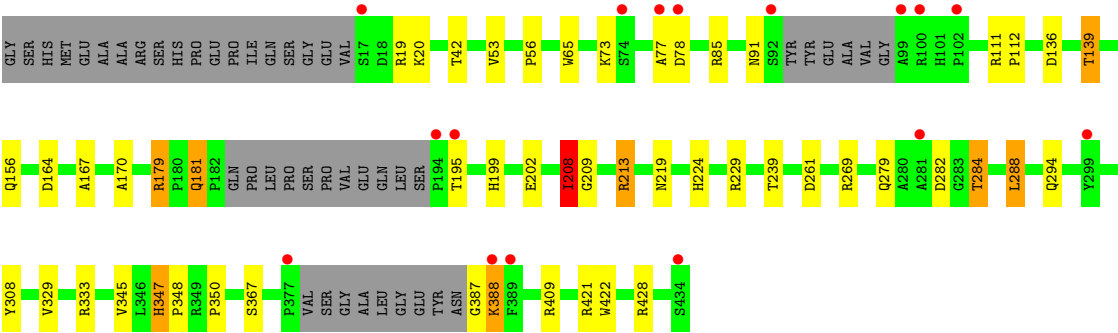
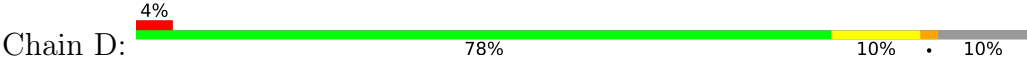


- Molecule 1: Uncharacterized protein





● Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.97Å 127.46Å 89.54Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.04 30.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.04) 98.4 (30.00-2.04)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.209 , 0.247 (Not available) , 0.214	Depositor DCC
R_{free} test set	5294 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12935	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: FE

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	1.35	15/3306 (0.5%)	1.47	15/4514 (0.3%)
1	B	1.46	18/3283 (0.5%)	1.49	17/4484 (0.4%)
1	C	1.31	11/3293 (0.3%)	1.45	17/4498 (0.4%)
1	D	1.32	10/3280 (0.3%)	1.47	17/4480 (0.4%)
All	All	1.36	54/13162 (0.4%)	1.47	66/17976 (0.4%)

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	B	1	1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	ARG	CA-CB	-31.94	0.99	1.53
1	D	347	HIS	CE1-NE2	10.60	1.43	1.32
1	A	213	ARG	CA-CB	-10.17	1.36	1.53
1	C	407	HIS	CE1-NE2	9.01	1.41	1.32
1	D	409	ARG	C-O	8.29	1.34	1.23
1	B	407	HIS	CE1-NE2	8.16	1.40	1.32
1	A	386	ASN	C-O	7.40	1.32	1.23
1	C	386	ASN	C-O	7.21	1.33	1.23
1	D	209	GLY	C-O	7.01	1.32	1.23
1	C	291	HIS	CE1-NE2	7.01	1.39	1.32
1	B	319	LYS	C-O	-6.94	1.16	1.24
1	B	202	GLU	C-O	6.90	1.32	1.23
1	C	421	ARG	C-O	6.88	1.33	1.24
1	B	292	GLY	C-O	6.86	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	213	ARG	C-O	-6.80	1.15	1.24
1	B	409	ARG	C-O	6.77	1.32	1.23
1	B	153	HIS	CE1-NE2	6.62	1.39	1.32
1	B	210	HIS	CE1-NE2	6.53	1.39	1.32
1	B	238	VAL	C-O	6.52	1.31	1.24
1	D	350	PRO	C-O	-6.43	1.16	1.23
1	A	292	GLY	C-O	6.29	1.32	1.23
1	A	302	VAL	C-O	6.25	1.31	1.24
1	B	41	GLU	C-O	6.21	1.32	1.23
1	A	41	GLU	C-O	6.18	1.32	1.23
1	A	409	ARG	C-O	6.14	1.31	1.23
1	D	167	ALA	C-O	-6.14	1.16	1.24
1	B	205	ARG	C-O	-6.13	1.16	1.24
1	A	84	PRO	C-O	-6.13	1.16	1.24
1	B	281	ALA	C-O	-6.00	1.16	1.24
1	B	269	ARG	C-O	-5.91	1.15	1.23
1	B	83	HIS	CE1-NE2	5.85	1.38	1.32
1	A	366	ALA	C-O	-5.75	1.16	1.24
1	C	49	PRO	C-O	-5.72	1.17	1.24
1	B	275	LEU	C-O	5.62	1.30	1.23
1	A	49	PRO	C-O	-5.57	1.17	1.24
1	C	109	LEU	C-O	5.56	1.30	1.23
1	D	202	GLU	C-O	5.55	1.30	1.23
1	A	373	PRO	C-O	-5.55	1.16	1.23
1	C	345	VAL	C-O	5.55	1.30	1.24
1	A	355	ALA	C-O	-5.46	1.17	1.24
1	B	174	LEU	C-O	-5.45	1.16	1.24
1	D	308	TYR	C-O	5.44	1.30	1.24
1	C	277	TRP	C-O	-5.42	1.17	1.23
1	A	152	HIS	CE1-NE2	5.40	1.38	1.32
1	A	145	PRO	C-O	-5.40	1.17	1.24
1	B	49	PRO	C-O	-5.37	1.17	1.24
1	A	347	HIS	CE1-NE2	5.33	1.37	1.32
1	C	426	GLY	C-O	5.31	1.31	1.23
1	B	320	ARG	C-O	5.27	1.30	1.23
1	A	230	PRO	C-O	-5.26	1.17	1.23
1	C	271	TRP	C-O	-5.15	1.17	1.23
1	D	269	ARG	C-O	-5.06	1.17	1.23
1	D	199	HIS	C-O	5.02	1.29	1.23
1	C	409	ARG	C-O	5.02	1.30	1.23

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	CB-CA-C	12.85	135.98	110.42
1	A	386	ASN	CA-C-N	11.39	132.53	120.00
1	A	386	ASN	C-N-CA	11.39	132.53	120.00
1	B	284	THR	CA-CB-OG1	-9.57	95.25	109.60
1	C	284	THR	CA-CB-OG1	-8.70	96.55	109.60
1	B	421	ARG	CG-CD-NE	-8.39	93.55	112.00
1	C	421	ARG	CG-CD-NE	-7.66	95.15	112.00
1	D	213	ARG	CA-C-O	-7.63	110.79	119.79
1	C	386	ASN	CA-C-N	6.99	135.12	121.41
1	C	386	ASN	C-N-CA	6.99	135.12	121.41
1	C	213	ARG	CG-CD-NE	6.92	127.22	112.00
1	A	212	GLY	O-C-N	6.91	128.62	122.88
1	A	421	ARG	CG-CD-NE	-6.90	96.81	112.00
1	D	421	ARG	CG-CD-NE	-6.75	97.14	112.00
1	D	333	ARG	CB-CG-CD	6.59	126.46	111.30
1	C	386	ASN	CA-CB-CG	6.54	119.14	112.60
1	C	387	GLY	CA-C-N	6.54	134.04	121.54
1	C	387	GLY	C-N-CA	6.54	134.04	121.54
1	A	208	ILE	CA-CB-CG2	6.17	120.99	110.50
1	B	387	GLY	CA-C-N	6.16	133.31	121.54
1	B	387	GLY	C-N-CA	6.16	133.31	121.54
1	D	208	ILE	CA-CB-CG2	6.15	120.95	110.50
1	A	42	THR	CA-CB-OG1	-6.09	100.46	109.60
1	B	208	ILE	CA-CB-CG2	6.07	120.81	110.50
1	B	213	ARG	CA-CB-CG	5.85	125.79	114.10
1	C	386	ASN	O-C-N	5.83	129.82	122.19
1	B	209	GLY	CA-C-O	-5.83	118.21	122.23
1	A	213	ARG	CB-CA-C	5.82	119.38	109.72
1	C	208	ILE	CA-CB-CG2	5.76	120.30	110.50
1	D	387	GLY	CA-C-N	5.75	132.51	121.54
1	D	387	GLY	C-N-CA	5.75	132.51	121.54
1	D	156	GLN	N-CA-C	-5.73	105.12	111.36
1	D	367	SER	CA-C-O	5.70	123.54	119.32
1	B	139	THR	CB-CA-C	5.68	121.97	110.38
1	D	213	ARG	CA-C-N	5.64	126.58	120.44
1	D	213	ARG	C-N-CA	5.64	126.58	120.44
1	C	42	THR	CA-CB-OG1	-5.63	101.15	109.60
1	A	284	THR	CA-CB-CG2	5.62	120.06	110.50
1	C	156	GLN	N-CA-C	-5.60	105.25	111.36
1	D	19	ARG	CB-CA-C	5.60	120.09	110.79
1	B	337	THR	CA-C-O	-5.55	115.34	121.33
1	A	213	ARG	N-CA-CB	5.41	118.00	109.83
1	D	42	THR	CA-CB-OG1	-5.38	101.53	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	CB-CA-C	5.36	115.96	109.85
1	D	219	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	367	SER	CA-C-O	5.28	123.23	119.32
1	C	87	ASP	CB-CA-C	5.28	119.17	110.88
1	A	172	ASN	CA-CB-CG	-5.27	107.33	112.60
1	D	85	ARG	CB-CG-CD	5.27	123.41	111.30
1	B	284	THR	CA-CB-CG2	5.26	119.45	110.50
1	A	178	TYR	CA-C-O	-5.25	115.49	121.00
1	A	386	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	17	SER	CA-C-N	5.19	129.72	121.99
1	A	17	SER	C-N-CA	5.19	129.72	121.99
1	C	91	ASN	CA-C-O	-5.11	115.95	121.87
1	C	213	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	D	428	ARG	N-CA-CB	-5.11	102.10	110.68
1	B	203	GLY	CA-C-O	-5.10	116.92	121.41
1	D	261	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	156	GLN	N-CA-C	-5.07	105.75	111.28
1	D	239	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	18	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	357	PHE	N-CA-C	-5.05	107.17	113.38
1	C	226	VAL	CA-C-O	-5.03	116.65	121.63
1	B	283	GLY	CA-C-N	5.02	129.35	120.87
1	B	283	GLY	C-N-CA	5.02	129.35	120.87

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	213	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	212	GLY	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	3193	0	3032	17	0
1	B	3170	0	3011	16	0
1	C	3180	0	3022	14	0
1	D	3167	0	3015	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	101	0	0	2	0
3	B	65	0	0	2	0
3	C	28	0	0	0	0
3	D	27	0	0	0	0
All	All	12935	0	12080	58	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 2.

All (58) 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:B:179:ARG:HH11	1:B:179:ARG:HG2	1.30	0.97
1:B:294:GLN:HG3	3:B:665:HOH:O	1.75	0.87
1:C:218:ASP:HB2	1:C:386:ASN:ND2	1.98	0.78
1:A:218:ASP:HB2	1:A:386:ASN:ND2	1.99	0.78
1:C:136:ASP:OD1	1:C:139:THR:HG23	1.85	0.76
1:B:179:ARG:NH1	3:B:601:HOH:O	2.09	0.74
1:D:136:ASP:OD1	1:D:139:THR:HG23	1.93	0.68
1:B:179:ARG:HH11	1:B:179:ARG:CG	2.06	0.67
1:B:180:PRO:O	1:B:182:PRO:HD3	1.95	0.65
1:B:23:GLN:OE1	1:B:129:GLU:OE1	2.15	0.64
1:C:170:ALA:HA	1:C:288:LEU:HD22	1.80	0.63
1:B:179:ARG:HG2	1:B:179:ARG:NH1	2.05	0.62
1:A:200:ILE:O	1:A:333:ARG:NH2	2.36	0.58
1:C:181:GLN:NE2	1:C:345:VAL:HG13	2.18	0.58
1:A:218:ASP:HB2	1:A:386:ASN:HD22	1.68	0.57
1:B:23:GLN:HG2	1:B:132:ILE:HG21	1.86	0.57
1:A:148:GLU:OE2	3:A:601:HOH:O	2.17	0.56
1:C:218:ASP:HB2	1:C:386:ASN:HD21	1.69	0.54
1:D:208:ILE:HG22	1:D:224:HIS:CE1	2.42	0.54
1:B:229:ARG:CZ	1:B:229:ARG:HB2	2.37	0.54
1:B:92:SER:O	1:B:100:ARG:NH1	2.39	0.54
1:A:156:GLN:NE2	1:A:385:TYR:OH	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLN:NE2	1:B:385:TYR:OH	2.42	0.53
1:C:208:ILE:HG22	1:C:224:HIS:CE1	2.44	0.53
1:A:181:GLN:NE2	1:A:345:VAL:HG13	2.24	0.52
1:A:208:ILE:HG22	1:A:224:HIS:CE1	2.45	0.52
1:B:208:ILE:HG22	1:B:224:HIS:CE1	2.44	0.52
1:A:282:ASP:OD1	1:A:284:THR:HB	2.09	0.51
1:C:156:GLN:NE2	1:C:385:TYR:OH	2.44	0.51
1:D:282:ASP:OD1	1:D:284:THR:HB	2.11	0.51
1:D:65:TRP:CZ2	1:D:91:ASN:HB2	2.46	0.51
1:A:111:ARG:HA	1:A:112:PRO:C	2.36	0.50
1:A:177:VAL:HG11	3:A:694:HOH:O	2.10	0.50
1:A:65:TRP:CZ2	1:A:91:ASN:HB2	2.47	0.49
1:B:282:ASP:OD1	1:B:284:THR:HB	2.13	0.49
1:A:23:GLN:HG3	1:A:132:ILE:HG21	1.95	0.49
1:C:111:ARG:HA	1:C:112:PRO:C	2.37	0.49
1:D:181:GLN:NE2	1:D:345:VAL:O	2.47	0.48
1:C:282:ASP:OD1	1:C:284:THR:HB	2.12	0.48
1:D:208:ILE:HD11	1:D:329:VAL:HG23	1.95	0.48
1:D:111:ARG:HA	1:D:112:PRO:C	2.40	0.47
1:C:23:GLN:HG3	1:C:132:ILE:HG21	1.97	0.47
1:B:111:ARG:HA	1:B:112:PRO:C	2.40	0.46
1:B:238:VAL:HB	1:B:427:VAL:HG13	1.97	0.45
1:B:65:TRP:CZ2	1:B:91:ASN:HB2	2.52	0.45
1:D:179:ARG:O	1:D:179:ARG:HG3	2.15	0.45
1:A:387:GLY:HA2	1:A:390:MET:SD	2.56	0.45
1:C:210:HIS:CE1	1:C:213:ARG:HB3	2.52	0.45
1:A:229:ARG:CZ	1:A:229:ARG:HB2	2.48	0.43
1:A:384:GLU:HG2	1:A:385:TYR:N	2.33	0.43
1:C:73:LYS:HD2	1:C:73:LYS:HA	1.81	0.42
1:D:347:HIS:CD2	1:D:348:PRO:HD2	2.55	0.42
1:D:170:ALA:HA	1:D:288:LEU:HD22	2.01	0.41
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.83	0.41
1:C:65:TRP:CZ2	1:C:91:ASN:HB2	2.56	0.41
1:A:347:HIS:CD2	1:A:348:PRO:HD2	2.55	0.41
1:D:53:VAL:HG13	1:D:164:ASP:HB3	2.04	0.40
1:C:275:LEU:HB3	1:C:304:HIS:HB3	2.04	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	387/437 (89%)	374 (97%)	11 (3%)	2 (0%)	24	16
1	B	384/437 (88%)	370 (96%)	11 (3%)	3 (1%)	16	9
1	C	385/437 (88%)	372 (97%)	9 (2%)	4 (1%)	12	6
1	D	384/437 (88%)	368 (96%)	14 (4%)	2 (0%)	24	16
All	All	1540/1748 (88%)	1484 (96%)	45 (3%)	11 (1%)	18	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	388	LYS
1	A	77	ALA
1	A	388	LYS
1	B	77	ALA
1	C	77	ALA
1	C	213	ARG
1	D	77	ALA
1	B	388	LYS
1	D	388	LYS
1	C	18	ASP
1	B	386	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	324/358 (90%)	313 (97%)	11 (3%)	32	27
1	B	321/358 (90%)	313 (98%)	8 (2%)	42	39
1	C	323/358 (90%)	309 (96%)	14 (4%)	26	20
1	D	322/358 (90%)	305 (95%)	17 (5%)	20	13
All	All	1290/1432 (90%)	1240 (96%)	50 (4%)	28	23

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	109	LEU
1	A	179	ARG
1	A	195	THR
1	A	208	ILE
1	A	213	ARG
1	A	279	GLN
1	A	284	THR
1	A	288	LEU
1	A	384	GLU
1	A	422	TRP
1	B	24	ARG
1	B	73	LYS
1	B	92	SER
1	B	179	ARG
1	B	208	ILE
1	B	284	THR
1	B	288	LEU
1	B	422	TRP
1	C	20	LYS
1	C	73	LYS
1	C	109	LEU
1	C	139	THR
1	C	179	ARG
1	C	208	ILE
1	C	213	ARG
1	C	279	GLN
1	C	288	LEU
1	C	294	GLN
1	C	352	SER
1	C	353	VAL
1	C	388	LYS
1	C	422	TRP

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Mol	Chain	Res	Type
1	D	20	LYS
1	D	56	PRO
1	D	73	LYS
1	D	78	ASP
1	D	139	THR
1	D	179	ARG
1	D	181	GLN
1	D	195	THR
1	D	208	ILE
1	D	213	ARG
1	D	229	ARG
1	D	279	GLN
1	D	284	THR
1	D	288	LEU
1	D	294	GLN
1	D	388	LYS
1	D	422	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	156	GLN
1	A	181	GLN
1	A	279	GLN
1	B	155	GLN
1	B	156	GLN
1	B	279	GLN
1	B	392	ASN
1	C	25	HIS
1	C	155	GLN
1	C	156	GLN
1	C	181	GLN
1	C	210	HIS
1	C	386	ASN
1	D	181	GLN
1	D	279	GLN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 4 are 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	395/437 (90%)	0.05	15 (3%)	44 44	20, 32, 65, 91	1 (0%)
1	B	392/437 (89%)	0.17	23 (5%)	28 28	20, 31, 70, 98	1 (0%)
1	C	393/437 (89%)	0.22	22 (5%)	30 30	23, 36, 70, 95	0
1	D	392/437 (89%)	0.15	16 (4%)	41 41	20, 33, 67, 103	1 (0%)
All	All	1572/1748 (89%)	0.15	76 (4%)	35 36	20, 33, 69, 103	3 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	VAL	5.2
1	B	377	PRO	4.7
1	B	99	ALA	4.3
1	C	353	VAL	4.2
1	C	386	ASN	4.1
1	D	194	PRO	4.1
1	B	385	TYR	4.1
1	D	377	PRO	3.9
1	C	99	ALA	3.8
1	C	377	PRO	3.8
1	C	195	THR	3.7
1	B	288	LEU	3.6
1	A	386	ASN	3.6
1	B	389	PHE	3.5
1	D	389	PHE	3.4
1	C	385	TYR	3.4
1	A	99	ALA	3.4
1	B	102	PRO	3.2
1	A	383	GLY	3.2
1	D	99	ALA	3.2
1	B	386	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	389	PHE	3.0
1	A	388	LYS	3.0
1	C	299	TYR	3.0
1	A	194	PRO	3.0
1	A	281	ALA	3.0
1	D	78	ASP	2.9
1	A	182	PRO	2.9
1	C	92	SER	2.9
1	D	299	TYR	2.9
1	D	77	ALA	2.9
1	C	387	GLY	2.8
1	D	195	THR	2.8
1	A	92	SER	2.7
1	B	133	ALA	2.7
1	C	288	LEU	2.7
1	C	303	CYS	2.7
1	C	76	LEU	2.7
1	C	182	PRO	2.7
1	B	388	LYS	2.7
1	C	104	PRO	2.7
1	B	17	SER	2.6
1	D	434	SER	2.6
1	D	388	LYS	2.6
1	A	80	ARG	2.6
1	C	100	ARG	2.6
1	B	21	ALA	2.6
1	C	17	SER	2.5
1	A	284	THR	2.5
1	C	388	LYS	2.5
1	C	77	ALA	2.4
1	B	22	TRP	2.4
1	A	385	TYR	2.4
1	C	101	HIS	2.4
1	C	376	ARG	2.4
1	B	434	SER	2.4
1	A	195	THR	2.3
1	A	282	ASP	2.3
1	D	74	SER	2.3
1	B	92	SER	2.2
1	C	281	ALA	2.2
1	B	134	HIS	2.2
1	B	136	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	283	GLY	2.2
1	B	80	ARG	2.2
1	B	140	TRP	2.2
1	D	102	PRO	2.1
1	D	100	ARG	2.1
1	D	92	SER	2.1
1	B	101	HIS	2.1
1	B	138	ARG	2.1
1	D	17	SER	2.1
1	C	102	PRO	2.1
1	D	281	ALA	2.1
1	B	73	LYS	2.0
1	B	131	PHE	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	FE	A	501	1/1	1.00	0.01	22,22,22,22	0
2	FE	B	501	1/1	1.00	0.01	30,30,30,30	0
2	FE	C	501	1/1	1.00	0.01	27,27,27,27	0
2	FE	D	501	1/1	1.00	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.