



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:25 pm BST

PDB ID : 5GS5
Title : Crystal structure of apo rat STING
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Li, L.F.; Jiang, Z.F.; Su, X.D.
Deposited on : 2016-08-13
Resolution : 1.84 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

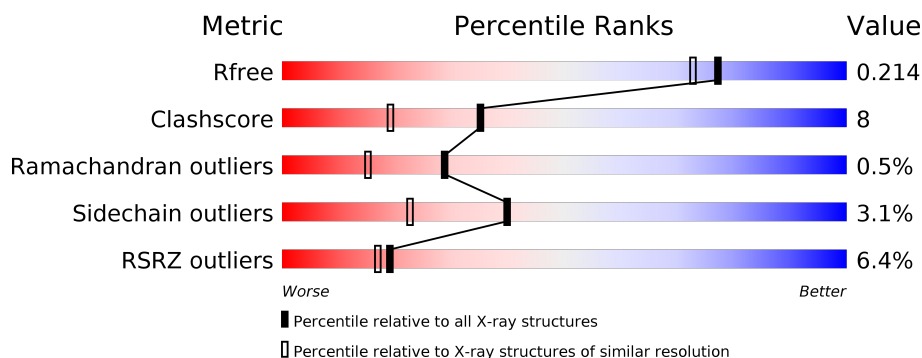
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 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	225	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	225	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	225	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	D	225	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• •</div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7224 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 Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1582	990	284	298	10			
1	B	205	Total	C	N	O	S	0	0	0
			1616	1010	289	307	10			
1	C	216	Total	C	N	O	S	0	0	0
			1698	1061	302	325	10			
1	D	213	Total	C	N	O	S	0	0	0
			1683	1052	299	322	10			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	MET	-	expression tag	UNP F1M391
A	118	GLY	-	expression tag	UNP F1M391
A	119	SER	-	expression tag	UNP F1M391
A	120	SER	-	expression tag	UNP F1M391
A	121	HIS	-	expression tag	UNP F1M391
A	122	HIS	-	expression tag	UNP F1M391
A	123	HIS	-	expression tag	UNP F1M391
A	124	HIS	-	expression tag	UNP F1M391
A	125	HIS	-	expression tag	UNP F1M391
A	126	HIS	-	expression tag	UNP F1M391
A	127	SER	-	expression tag	UNP F1M391
A	128	SER	-	expression tag	UNP F1M391
A	129	GLY	-	expression tag	UNP F1M391
A	130	GLU	-	expression tag	UNP F1M391
A	131	ASN	-	expression tag	UNP F1M391
A	132	LEU	-	expression tag	UNP F1M391
A	133	TYR	-	expression tag	UNP F1M391
A	134	PHE	-	expression tag	UNP F1M391
A	135	GLN	-	expression tag	UNP F1M391
A	136	GLY	-	expression tag	UNP F1M391
A	137	SER	-	expression tag	UNP F1M391

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Chain	Residue	Modelled	Actual	Comment	Reference
A	138	HIS	-	expression tag	UNP F1M391
A	139	MET	-	expression tag	UNP F1M391
A	338	ALA	-	expression tag	UNP F1M391
A	339	ALA	-	expression tag	UNP F1M391
A	340	ALA	-	expression tag	UNP F1M391
A	341	ALA	-	expression tag	UNP F1M391
B	117	MET	-	expression tag	UNP F1M391
B	118	GLY	-	expression tag	UNP F1M391
B	119	SER	-	expression tag	UNP F1M391
B	120	SER	-	expression tag	UNP F1M391
B	121	HIS	-	expression tag	UNP F1M391
B	122	HIS	-	expression tag	UNP F1M391
B	123	HIS	-	expression tag	UNP F1M391
B	124	HIS	-	expression tag	UNP F1M391
B	125	HIS	-	expression tag	UNP F1M391
B	126	HIS	-	expression tag	UNP F1M391
B	127	SER	-	expression tag	UNP F1M391
B	128	SER	-	expression tag	UNP F1M391
B	129	GLY	-	expression tag	UNP F1M391
B	130	GLU	-	expression tag	UNP F1M391
B	131	ASN	-	expression tag	UNP F1M391
B	132	LEU	-	expression tag	UNP F1M391
B	133	TYR	-	expression tag	UNP F1M391
B	134	PHE	-	expression tag	UNP F1M391
B	135	GLN	-	expression tag	UNP F1M391
B	136	GLY	-	expression tag	UNP F1M391
B	137	SER	-	expression tag	UNP F1M391
B	138	HIS	-	expression tag	UNP F1M391
B	139	MET	-	expression tag	UNP F1M391
B	338	ALA	-	expression tag	UNP F1M391
B	339	ALA	-	expression tag	UNP F1M391
B	340	ALA	-	expression tag	UNP F1M391
B	341	ALA	-	expression tag	UNP F1M391
C	117	MET	-	expression tag	UNP F1M391
C	118	GLY	-	expression tag	UNP F1M391
C	119	SER	-	expression tag	UNP F1M391
C	120	SER	-	expression tag	UNP F1M391
C	121	HIS	-	expression tag	UNP F1M391
C	122	HIS	-	expression tag	UNP F1M391
C	123	HIS	-	expression tag	UNP F1M391
C	124	HIS	-	expression tag	UNP F1M391
C	125	HIS	-	expression tag	UNP F1M391

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Chain	Residue	Modelled	Actual	Comment	Reference
C	126	HIS	-	expression tag	UNP F1M391
C	127	SER	-	expression tag	UNP F1M391
C	128	SER	-	expression tag	UNP F1M391
C	129	GLY	-	expression tag	UNP F1M391
C	130	GLU	-	expression tag	UNP F1M391
C	131	ASN	-	expression tag	UNP F1M391
C	132	LEU	-	expression tag	UNP F1M391
C	133	TYR	-	expression tag	UNP F1M391
C	134	PHE	-	expression tag	UNP F1M391
C	135	GLN	-	expression tag	UNP F1M391
C	136	GLY	-	expression tag	UNP F1M391
C	137	SER	-	expression tag	UNP F1M391
C	138	HIS	-	expression tag	UNP F1M391
C	139	MET	-	expression tag	UNP F1M391
C	338	ALA	-	expression tag	UNP F1M391
C	339	ALA	-	expression tag	UNP F1M391
C	340	ALA	-	expression tag	UNP F1M391
C	341	ALA	-	expression tag	UNP F1M391
D	117	MET	-	expression tag	UNP F1M391
D	118	GLY	-	expression tag	UNP F1M391
D	119	SER	-	expression tag	UNP F1M391
D	120	SER	-	expression tag	UNP F1M391
D	121	HIS	-	expression tag	UNP F1M391
D	122	HIS	-	expression tag	UNP F1M391
D	123	HIS	-	expression tag	UNP F1M391
D	124	HIS	-	expression tag	UNP F1M391
D	125	HIS	-	expression tag	UNP F1M391
D	126	HIS	-	expression tag	UNP F1M391
D	127	SER	-	expression tag	UNP F1M391
D	128	SER	-	expression tag	UNP F1M391
D	129	GLY	-	expression tag	UNP F1M391
D	130	GLU	-	expression tag	UNP F1M391
D	131	ASN	-	expression tag	UNP F1M391
D	132	LEU	-	expression tag	UNP F1M391
D	133	TYR	-	expression tag	UNP F1M391
D	134	PHE	-	expression tag	UNP F1M391
D	135	GLN	-	expression tag	UNP F1M391
D	136	GLY	-	expression tag	UNP F1M391
D	137	SER	-	expression tag	UNP F1M391
D	138	HIS	-	expression tag	UNP F1M391
D	139	MET	-	expression tag	UNP F1M391
D	338	ALA	-	expression tag	UNP F1M391

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Chain	Residue	Modelled	Actual	Comment	Reference
D	339	ALA	-	expression tag	UNP F1M391
D	340	ALA	-	expression tag	UNP F1M391
D	341	ALA	-	expression tag	UNP F1M391

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

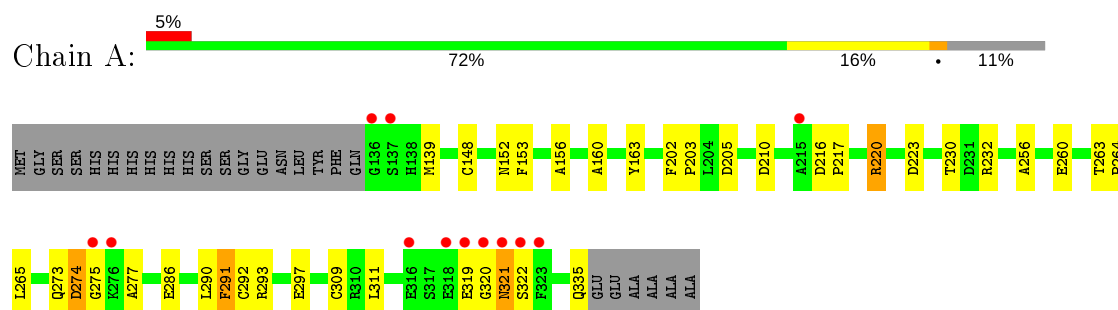
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	139	Total 139	O 139	0	0
3	B	152	Total 152	O 152	0	0
3	C	147	Total 147	O 147	0	0
3	D	162	Total 162	O 162	0	0

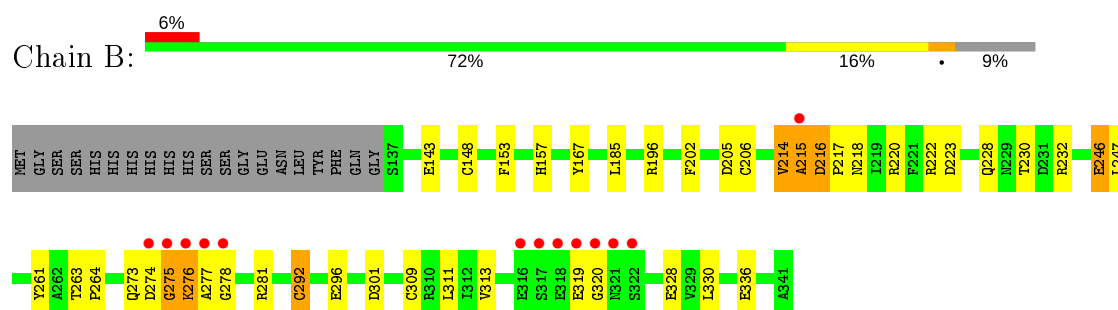
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

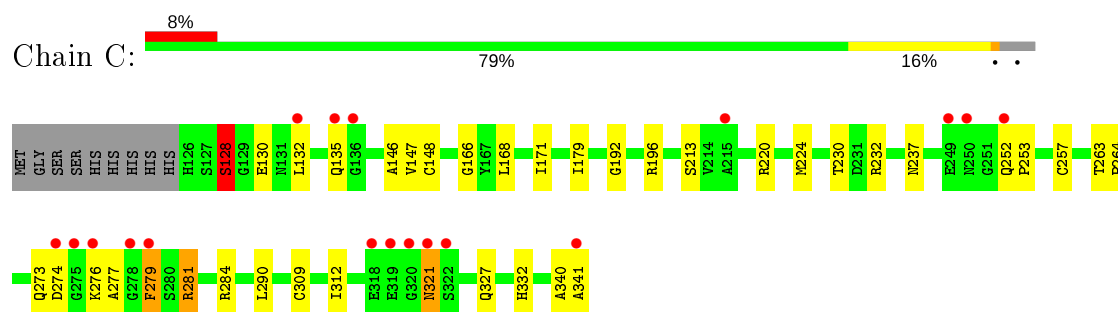
- Molecule 1: Stimulator of interferon genes protein



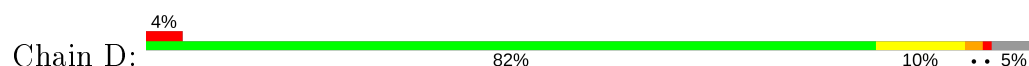
- Molecule 1: Stimulator of interferon genes protein

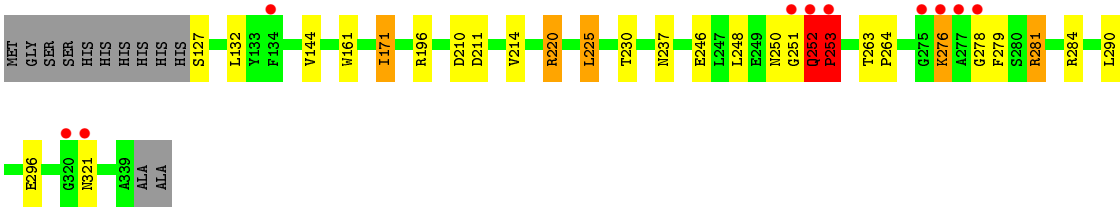


- Molecule 1: Stimulator of interferon genes protein



- Molecule 1: Stimulator of interferon genes protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.29Å 75.51Å 87.64Å 90.00° 115.35° 90.00°	Depositor
Resolution (Å)	42.73 – 1.84 45.39 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.73-1.84) 99.0 (45.39-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.181 , 0.222 0.190 , 0.214	Depositor DCC
R_{free} test set	3531 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7224	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.98% 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: SO4

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	1.60	7/1613 (0.4%)	0.89	1/2180 (0.0%)
1	B	1.72	12/1647 (0.7%)	0.91	5/2227 (0.2%)
1	C	1.60	5/1731 (0.3%)	0.90	4/2340 (0.2%)
1	D	1.79	3/1716 (0.2%)	1.02	8/2319 (0.3%)
All	All	1.68	27/6707 (0.4%)	0.93	18/9066 (0.2%)

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	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	253	PRO	N-CD	30.03	1.89	1.47
1	B	167	TYR	N-CA	-10.81	1.24	1.46
1	A	309	CYS	CB-SG	-8.90	1.67	1.82
1	A	292	CYS	CB-SG	-7.93	1.68	1.82
1	B	261	TYR	CD2-CE2	-7.44	1.28	1.39
1	C	309	CYS	CB-SG	-7.01	1.70	1.82
1	B	336	GLU	CD-OE2	-6.45	1.18	1.25
1	B	292	CYS	CB-SG	-6.42	1.71	1.82
1	C	146	ALA	CA-CB	-6.22	1.39	1.52
1	B	309	CYS	CB-SG	-6.18	1.71	1.82
1	B	328	GLU	CD-OE2	-6.13	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	261	TYR	CE1-CZ	-5.82	1.30	1.38
1	B	246	GLU	CB-CG	-5.63	1.41	1.52
1	B	214	VAL	CB-CG1	-5.61	1.41	1.52
1	A	286	GLU	CB-CG	-5.50	1.41	1.52
1	B	206	CYS	CB-SG	-5.50	1.72	1.81
1	D	161	TRP	C-O	-5.43	1.13	1.23
1	B	143	GLU	CD-OE2	-5.39	1.19	1.25
1	A	260	GLU	CD-OE2	-5.37	1.19	1.25
1	C	166	GLY	C-O	-5.25	1.15	1.23
1	C	257	CYS	CB-SG	-5.24	1.73	1.81
1	B	313	VAL	CB-CG1	-5.22	1.41	1.52
1	D	279	PHE	CD1-CE1	-5.20	1.28	1.39
1	A	256	ALA	CA-CB	-5.17	1.41	1.52
1	C	279	PHE	CD2-CE2	-5.04	1.29	1.39
1	A	163	TYR	CD2-CE2	-5.02	1.31	1.39
1	A	291	PHE	CE1-CZ	-5.01	1.27	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	PRO	CA-N-CD	-16.18	88.85	111.50
1	D	253	PRO	N-CA-C	8.03	132.98	112.10
1	D	252	GLN	N-CA-C	-7.41	91.00	111.00
1	A	274	ASP	N-CA-C	-7.27	91.38	111.00
1	B	167	TYR	N-CA-C	7.25	130.56	111.00
1	B	319	GLU	N-CA-C	-7.11	91.81	111.00
1	B	320	GLY	N-CA-C	-6.79	96.12	113.10
1	D	225	LEU	CB-CG-CD1	6.74	122.46	111.00
1	C	281	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	253	PRO	N-CD-CG	-6.62	93.27	103.20
1	D	220	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	281	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	253	PRO	N-CA-CB	-6.10	95.89	102.60
1	C	232	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	D	281	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	128	SER	CA-C-N	5.39	126.99	116.20
1	B	281	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	277	ALA	N-CA-CB	-5.04	103.05	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	276	LYS	Peptide
1	C	128	SER	Peptide
1	D	250	ASN	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	1582	0	1547	23	1
1	B	1616	0	1576	37	0
1	C	1698	0	1643	23	1
1	D	1683	0	1631	30	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
3	A	139	0	0	4	0
3	B	152	0	0	4	0
3	C	147	0	0	3	0
3	D	162	0	0	6	0
All	All	7224	0	6397	107	1

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 8.

All (107) 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:253:PRO:N	1:D:253:PRO:CD	1.89	1.28
1:B:274:ASP:CG	1:B:276:LYS:HD3	1.57	1.24
1:B:274:ASP:OD1	1:B:276:LYS:HD3	1.41	1.16
1:B:153:PHE:HZ	1:B:278:GLY:HA3	1.21	1.03
1:B:274:ASP:OD1	1:B:276:LYS:CD	2.07	1.01
1:B:274:ASP:O	1:B:276:LYS:N	1.94	1.00
1:D:252:GLN:HB3	1:D:253:PRO:HD3	1.41	0.98
1:B:230:THR:HG22	1:B:232:ARG:H	1.29	0.97
1:D:252:GLN:HB3	1:D:253:PRO:CD	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASP:O	1:B:276:LYS:HD2	1.69	0.93
1:A:230:THR:HG22	1:A:232:ARG:H	1.35	0.91
1:D:230:THR:HG23	1:D:237:ASN:OD1	1.71	0.91
1:B:153:PHE:CZ	1:B:278:GLY:HA3	2.07	0.90
1:D:251:GLY:O	3:D:501:HOH:O	1.93	0.86
1:B:274:ASP:O	1:B:276:LYS:CD	2.25	0.83
1:C:327:GLN:HE21	1:D:321:ASN:HD21	1.29	0.80
1:C:281:ARG:HD3	1:C:284:ARG:NH2	1.97	0.79
1:A:275:GLY:HA2	3:A:501:HOH:O	1.82	0.79
1:B:215:ALA:HA	1:B:216:ASP:HB3	1.69	0.75
1:C:327:GLN:NE2	1:D:321:ASN:HD21	1.84	0.74
1:C:230:THR:HG23	1:C:237:ASN:OD1	1.88	0.74
1:B:214:VAL:O	1:B:215:ALA:HB3	1.90	0.72
1:B:274:ASP:CB	1:B:276:LYS:HD3	2.22	0.68
1:C:281:ARG:HD3	1:C:284:ARG:HH22	1.57	0.67
1:A:320:GLY:C	1:A:321:ASN:OD1	2.34	0.65
1:C:274:ASP:O	1:C:277:ALA:HB3	1.98	0.64
1:B:214:VAL:O	1:B:215:ALA:CB	2.46	0.63
1:B:214:VAL:HG12	1:B:215:ALA:N	2.12	0.62
1:B:222:ARG:NH2	1:B:246:GLU:OE1	2.34	0.61
1:B:215:ALA:HA	1:B:216:ASP:CB	2.28	0.60
1:C:312:ILE:HG23	1:C:332:HIS:CE1	2.37	0.59
1:B:296:GLU:HG3	1:B:311:LEU:HD12	1.84	0.59
1:A:321:ASN:OD1	1:A:321:ASN:N	2.32	0.59
1:B:157:HIS:HB2	3:B:505:HOH:O	2.02	0.58
1:A:319:GLU:HA	1:A:319:GLU:OE1	2.04	0.58
1:A:152:ASN:OD1	1:A:152:ASN:C	2.41	0.57
1:B:228:GLN:HB2	1:B:230:THR:OG1	2.05	0.56
1:B:214:VAL:HG12	1:B:215:ALA:H	1.70	0.56
1:C:192:GLY:HA2	3:C:582:HOH:O	2.06	0.56
1:D:252:GLN:NE2	1:D:252:GLN:HA	2.21	0.56
1:D:252:GLN:C	1:D:253:PRO:CD	2.71	0.55
1:A:202:PHE:CE2	1:A:311:LEU:HD22	2.42	0.55
1:B:274:ASP:HB3	1:B:276:LYS:HG2	1.89	0.55
1:C:340:ALA:O	1:C:341:ALA:HB3	2.08	0.54
1:C:213:SER:HB3	1:C:220:ARG:HH12	1.74	0.52
1:A:156:ALA:HB3	1:A:290:LEU:HD23	1.91	0.52
1:D:246:GLU:CD	1:D:253:PRO:HB3	2.31	0.52
1:B:217:PRO:HG2	1:C:253:PRO:O	2.11	0.51
1:D:263:THR:HB	1:D:264:PRO:HD3	1.91	0.51
1:B:222:ARG:NE	1:B:246:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLU:CD	1:D:253:PRO:CB	2.79	0.51
1:A:335:GLN:C	3:A:509:HOH:O	2.49	0.51
1:A:202:PHE:HE2	1:A:311:LEU:HD22	1.76	0.50
1:A:321:ASN:CG	1:A:322:SER:H	2.14	0.50
1:C:340:ALA:O	1:C:341:ALA:CB	2.59	0.50
1:D:248:LEU:HD22	1:D:252:GLN:C	2.31	0.49
1:C:263:THR:HB	1:C:264:PRO:HD3	1.93	0.49
1:D:276:LYS:O	1:D:278:GLY:N	2.46	0.49
1:A:210:ASP:HB3	3:A:606:HOH:O	2.13	0.49
1:B:274:ASP:O	1:B:275:GLY:C	2.45	0.48
1:B:273:GLN:O	1:B:275:GLY:N	2.46	0.47
1:A:205:ASP:HB2	3:A:585:HOH:O	2.14	0.47
1:B:202:PHE:CE1	1:B:292:CYS:HB2	2.49	0.47
1:D:132:LEU:HD21	3:D:639:HOH:O	2.15	0.47
1:D:281:ARG:NE	1:D:284:ARG:HH22	2.13	0.47
1:B:196:ARG:HD3	3:B:556:HOH:O	2.14	0.47
1:B:185:LEU:CD2	1:D:296:GLU:HB3	2.45	0.46
1:A:160:ALA:HA	1:A:291:PHE:HE1	1.80	0.46
1:A:273:GLN:O	1:A:275:GLY:N	2.48	0.46
1:B:274:ASP:OD1	1:B:276:LYS:HD2	2.09	0.46
1:D:196:ARG:HD3	3:D:590:HOH:O	2.15	0.46
1:C:273:GLN:HG3	3:C:637:HOH:O	2.15	0.46
1:A:139:MET:HE1	1:C:263:THR:HA	1.97	0.46
1:D:210:ASP:HA	3:D:603:HOH:O	2.14	0.46
1:D:276:LYS:C	1:D:278:GLY:N	2.69	0.46
1:D:281:ARG:HD3	3:D:633:HOH:O	2.15	0.45
1:A:220:ARG:HH11	1:A:220:ARG:HG2	1.81	0.45
1:D:144:VAL:O	1:D:144:VAL:HG22	2.17	0.45
1:D:252:GLN:NE2	1:D:252:GLN:CA	2.80	0.45
1:A:203:PRO:HD2	1:A:265:LEU:CD1	2.48	0.44
1:C:132:LEU:HB2	3:C:562:HOH:O	2.17	0.44
1:D:253:PRO:HD2	1:D:253:PRO:O	2.17	0.44
1:A:274:ASP:O	1:A:277:ALA:HB3	2.18	0.43
1:B:153:PHE:CZ	1:B:278:GLY:CA	2.90	0.43
1:A:152:ASN:OD1	1:A:152:ASN:O	2.37	0.43
1:B:205:ASP:HB2	3:B:607:HOH:O	2.18	0.43
1:A:320:GLY:CA	1:A:321:ASN:OD1	2.67	0.43
1:D:246:GLU:CD	1:D:253:PRO:HB2	2.40	0.42
1:D:281:ARG:NH2	3:D:513:HOH:O	2.51	0.42
1:B:218:ASN:ND2	3:B:506:HOH:O	2.43	0.42
1:B:247:LEU:HD13	1:B:330:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:O	1:D:171:ILE:HD13	2.20	0.42
1:B:216:ASP:H	1:C:252:GLN:HE22	1.66	0.42
1:C:168:LEU:HA	1:C:171:ILE:HG22	2.01	0.42
1:B:274:ASP:O	1:B:276:LYS:CG	2.67	0.42
1:B:220:ARG:HH11	1:B:220:ARG:HD3	1.73	0.41
1:C:147:VAL:O	1:C:148:CYS:HB3	2.20	0.41
1:C:179:ILE:HD13	1:C:196:ARG:HA	2.03	0.41
1:C:321:ASN:N	1:C:321:ASN:OD1	2.52	0.41
1:B:263:THR:N	1:B:264:PRO:CD	2.84	0.41
1:C:252:GLN:HA	1:C:253:PRO:HD3	1.95	0.41
1:D:263:THR:N	1:D:264:PRO:CD	2.83	0.41
1:C:128:SER:HB2	1:C:130:GLU:H	1.86	0.41
1:D:211:ASP:HB3	1:D:214:VAL:HG23	2.02	0.41
1:A:263:THR:N	1:A:264:PRO:CD	2.85	0.40
1:D:248:LEU:HD23	1:D:253:PRO:HA	2.03	0.40
1:A:216:ASP:OD1	1:A:217:PRO:HD2	2.21	0.40

All (1) 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)
1:A:297:GLU:OE1	1:C:135:GLN:OE1[4_445]	1.22	0.98

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	198/225 (88%)	194 (98%)	3 (2%)	1 (0%)	29	15
1	B	203/225 (90%)	197 (97%)	3 (2%)	3 (2%)	10	2
1	C	214/225 (95%)	208 (97%)	6 (3%)	0	100	100
1	D	211/225 (94%)	205 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	826/900 (92%)	804 (97%)	18 (2%)	4 (0%)	29	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	ASN
1	B	275	GLY
1	B	216	ASP
1	B	215	ALA

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	170/189 (90%)	165 (97%)	5 (3%)	42	25
1	B	172/189 (91%)	169 (98%)	3 (2%)	60	47
1	C	180/189 (95%)	174 (97%)	6 (3%)	38	20
1	D	180/189 (95%)	172 (96%)	8 (4%)	28	11
All	All	702/756 (93%)	680 (97%)	22 (3%)	40	23

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	CYS
1	A	153	PHE
1	A	220	ARG
1	A	223	ASP
1	A	293	ARG
1	B	148	CYS
1	B	223	ASP
1	B	301	ASP
1	C	128	SER
1	C	224	MET
1	C	276	LYS

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Mol	Chain	Res	Type
1	C	279	PHE
1	C	290	LEU
1	C	321	ASN
1	D	127	SER
1	D	171	ILE
1	D	220	ARG
1	D	225	LEU
1	D	252	GLN
1	D	253	PRO
1	D	276	LYS
1	D	290	LEU

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

Mol	Chain	Res	Type
1	A	327	GLN
1	C	252	GLN
1	C	327	GLN
1	D	135	GLN
1	D	252	GLN

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](#)

9 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	D	403	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	C	403	-	4,4,4	0.19	0	6,6,6	0.11	0
2	SO4	D	402	-	4,4,4	0.24	0	6,6,6	0.49	0
2	SO4	B	401	-	4,4,4	0.15	0	6,6,6	0.26	0
2	SO4	C	401	-	4,4,4	0.11	0	6,6,6	0.37	0
2	SO4	D	401	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	A	402	-	4,4,4	0.16	0	6,6,6	0.24	0
2	SO4	C	402	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	A	401	-	4,4,4	0.19	0	6,6,6	0.48	0

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	200/225 (88%)	0.14	12 (6%) 21 19	12, 22, 56, 88	0
1	B	205/225 (91%)	0.04	13 (6%) 20 17	10, 20, 51, 84	0
1	C	216/225 (96%)	0.34	18 (8%) 11 10	12, 24, 59, 91	0
1	D	213/225 (94%)	0.12	10 (4%) 31 28	11, 21, 50, 88	0
All	All	834/900 (92%)	0.16	53 (6%) 19 17	10, 22, 55, 91	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	GLN	9.0
1	A	319	GLU	7.0
1	D	275	GLY	6.5
1	D	253	PRO	6.2
1	D	321	ASN	5.6
1	C	321	ASN	5.5
1	A	322	SER	5.3
1	A	215	ALA	5.1
1	D	278	GLY	5.0
1	C	278	GLY	4.9
1	C	275	GLY	4.9
1	B	277	ALA	4.7
1	C	322	SER	4.7
1	A	321	ASN	4.6
1	B	215	ALA	4.0
1	B	275	GLY	3.8
1	B	276	LYS	3.6
1	C	320	GLY	3.6
1	C	276	LYS	3.5
1	C	132	LEU	3.4
1	C	341	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	320	GLY	3.3
1	A	320	GLY	3.3
1	C	250	ASN	3.2
1	A	316	GLU	3.2
1	B	319	GLU	3.1
1	B	316	GLU	2.9
1	C	136	GLY	2.9
1	B	274	ASP	2.8
1	C	318	GLU	2.8
1	D	251	GLY	2.7
1	C	274	ASP	2.7
1	A	275	GLY	2.7
1	A	136	GLY	2.6
1	C	249	GLU	2.6
1	D	277	ALA	2.6
1	A	318	GLU	2.5
1	A	323	PHE	2.5
1	B	322	SER	2.5
1	B	317	SER	2.4
1	B	278	GLY	2.4
1	B	321	ASN	2.4
1	D	320	GLY	2.4
1	C	215	ALA	2.3
1	C	319	GLU	2.3
1	A	276	LYS	2.2
1	C	135	GLN	2.2
1	C	252	GLN	2.2
1	B	318	GLU	2.1
1	D	134	PHE	2.1
1	A	137	SER	2.0
1	C	279	PHE	2.0
1	D	276	LYS	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 ⓘ

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. 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	SO4	D	401	5/5	0.94	0.16	53,53,57,58	0
2	SO4	C	403	5/5	0.95	0.13	34,38,45,48	0
2	SO4	D	403	5/5	0.95	0.18	37,46,50,54	0
2	SO4	B	401	5/5	0.97	0.12	36,43,51,51	0
2	SO4	D	402	5/5	0.97	0.09	23,24,26,26	0
2	SO4	C	401	5/5	0.99	0.09	16,17,22,29	0
2	SO4	A	402	5/5	0.99	0.08	21,22,27,29	0
2	SO4	C	402	5/5	0.99	0.11	24,26,30,34	0
2	SO4	A	401	5/5	0.99	0.09	13,16,19,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.