



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 25, 2017 – 11:19 am GMT

PDB ID : 5A5K  
Title : AtGSTF2 from Arabidopsis thaliana in complex with camalexin  
Authors : Ahmad, L.; Rylott, E.; Bruce, N.C.; Edwards, R.; Grogan, G.  
Deposited on : 2015-06-18  
Resolution : 2.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	recalc29047
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc29047

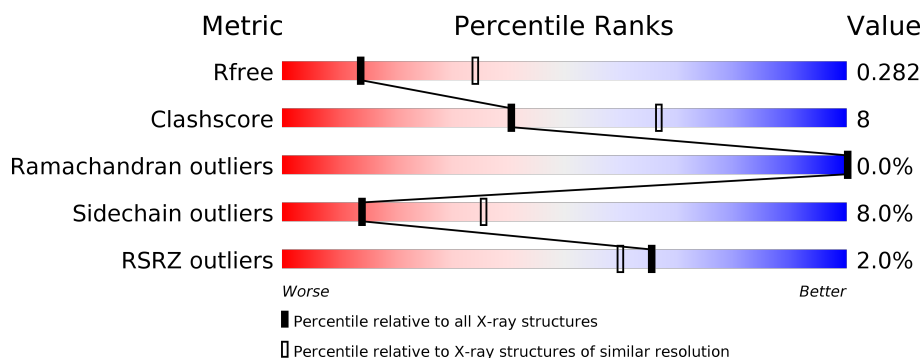
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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))
$R_{free}$	100719	3276 (2.80-2.76)
Clashscore	112137	3771 (2.80-2.76)
Ramachandran outliers	110173	3707 (2.80-2.76)
Sidechain outliers	110143	3709 (2.80-2.76)
RSRZ outliers	101464	3307 (2.80-2.76)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	212	<div> <div style="width: 79%;"></div> <div style="width: 17%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> </div>
1	B	212	<div> <div style="width: 79%;"></div> <div style="width: 17%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> </div>
1	C	212	<div> <div style="width: 83%;"></div> <div style="width: 14%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div>
1	D	212	<div> <div style="width: 2%;"></div> <div style="width: 78%;"></div> <div style="width: 16%;"></div> <div style="width: 4%;"></div> </div>
1	E	212	<div> <div style="width: 5%;"></div> <div style="width: 82%;"></div> <div style="width: 12%;"></div> <div style="width: 3%;"></div> </div>
1	F	212	<div> <div style="width: 84%;"></div> <div style="width: 10%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	212	
1	H	212	
1	I	212	
1	J	212	
1	K	212	
1	L	212	
1	M	212	
1	N	212	
1	O	212	
1	P	212	
1	Q	212	
1	R	212	
1	S	212	
1	T	212	
1	U	212	
1	V	212	
1	W	212	
1	X	212	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	7WB	T	1212	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39024 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 GLUTATHIONE S-TRANSFERASE F2.

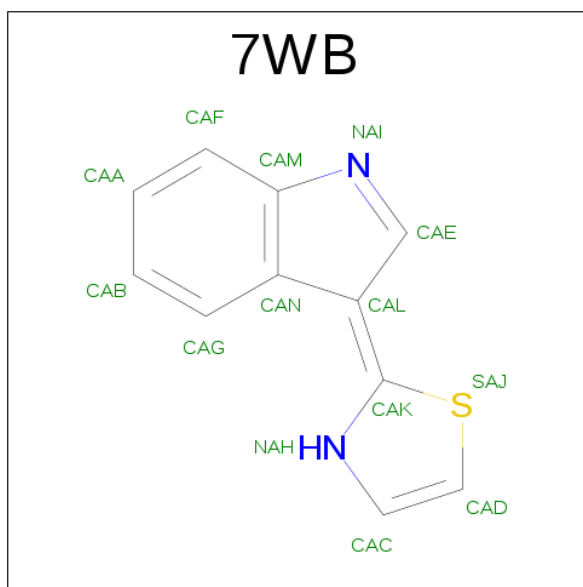
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1602	1035	272	293	2			
1	B	210	Total	C	N	O	S	0	1	0
			1650	1058	280	310	2			
1	C	210	Total	C	N	O	S	0	0	0
			1610	1038	271	299	2			
1	D	209	Total	C	N	O	S	0	0	0
			1589	1021	268	298	2			
1	E	210	Total	C	N	O	S	0	0	0
			1553	999	266	286	2			
1	F	210	Total	C	N	O	S	0	0	0
			1609	1037	274	296	2			
1	G	210	Total	C	N	O	S	0	1	0
			1543	991	266	284	2			
1	H	210	Total	C	N	O	S	0	0	0
			1515	962	260	291	2			
1	I	210	Total	C	N	O	S	0	0	0
			1644	1056	278	308	2			
1	J	210	Total	C	N	O	S	0	0	0
			1640	1054	276	308	2			
1	K	210	Total	C	N	O	S	0	0	0
			1635	1052	276	305	2			
1	L	210	Total	C	N	O	S	0	0	0
			1645	1058	277	308	2			
1	M	210	Total	C	N	O	S	0	0	0
			1642	1057	275	308	2			
1	N	204	Total	C	N	O	S	0	0	0
			1501	968	255	276	2			
1	O	203	Total	C	N	O	S	0	0	0
			1461	944	249	266	2			
1	P	210	Total	C	N	O	S	0	0	0
			1615	1037	272	304	2			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	210	Total	C	N	O	S	0	0	0
			1619	1041	272	304	2			
1	R	210	Total	C	N	O	S	0	0	0
			1625	1047	277	299	2			
1	S	210	Total	C	N	O	S	0	0	0
			1653	1060	280	311	2			
1	T	206	Total	C	N	O	S	0	0	0
			1473	943	249	279	2			
1	U	210	Total	C	N	O	S	0	0	0
			1644	1057	281	304	2			
1	V	210	Total	C	N	O	S	0	0	0
			1632	1047	277	306	2			
1	W	210	Total	C	N	O	S	0	0	0
			1639	1051	278	308	2			
1	X	210	Total	C	N	O	S	0	0	0
			1645	1059	277	307	2			

- Molecule 2 is (2Z)-2-indol-3-ylidene-3H-1,3-thiazole (three-letter code: 7WB) (formula: C<sub>11</sub>H<sub>8</sub>N<sub>2</sub>S<sub>1</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			14	11	2	1		
2	B	1	Total	C	N	S	0	0
			14	11	2	1		
2	C	1	Total	C	N	S	0	0
			14	11	2	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	S	0	0
			14	11	2	1		
2	E	1	Total	C	N	S	0	0
			14	11	2	1		
2	F	1	Total	C	N	S	0	0
			14	11	2	1		
2	G	1	Total	C	N	S	0	0
			14	11	2	1		
2	H	1	Total	C	N	S	0	0
			14	11	2	1		
2	I	1	Total	C	N	S	0	0
			14	11	2	1		
2	J	1	Total	C	N	S	0	0
			14	11	2	1		
2	K	1	Total	C	N	S	0	0
			14	11	2	1		
2	L	1	Total	C	N	S	0	0
			14	11	2	1		
2	M	1	Total	C	N	S	0	0
			14	11	2	1		
2	N	1	Total	C	N	S	0	0
			14	11	2	1		
2	O	1	Total	C	N	S	0	0
			14	11	2	1		
2	P	1	Total	C	N	S	0	0
			14	11	2	1		
2	Q	1	Total	C	N	S	0	0
			14	11	2	1		
2	R	1	Total	C	N	S	0	0
			14	11	2	1		
2	S	1	Total	C	N	S	0	0
			14	11	2	1		
2	T	1	Total	C	N	S	0	0
			14	11	2	1		
2	U	1	Total	C	N	S	0	0
			14	11	2	1		
2	V	1	Total	C	N	S	0	0
			14	11	2	1		
2	W	1	Total	C	N	S	0	0
			14	11	2	1		
2	X	1	Total	C	N	S	0	0
			14	11	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0
3	B	15	Total O 15 15	0	0
3	C	13	Total O 13 13	0	0
3	D	15	Total O 15 15	0	0
3	E	19	Total O 19 19	0	0
3	F	10	Total O 10 10	0	0
3	G	13	Total O 13 13	0	0
3	H	6	Total O 6 6	0	0
3	I	15	Total O 15 15	0	0
3	J	22	Total O 22 22	0	0
3	K	13	Total O 13 13	0	0
3	L	13	Total O 13 13	0	0
3	M	15	Total O 15 15	0	0
3	N	9	Total O 9 9	0	0
3	O	7	Total O 7 7	0	0
3	P	9	Total O 9 9	0	0
3	Q	9	Total O 9 9	0	0
3	R	3	Total O 3 3	0	0
3	S	13	Total O 13 13	0	0
3	T	4	Total O 4 4	0	0
3	U	20	Total O 20 20	0	0

*Continued on next page...*

*Continued from previous page...*

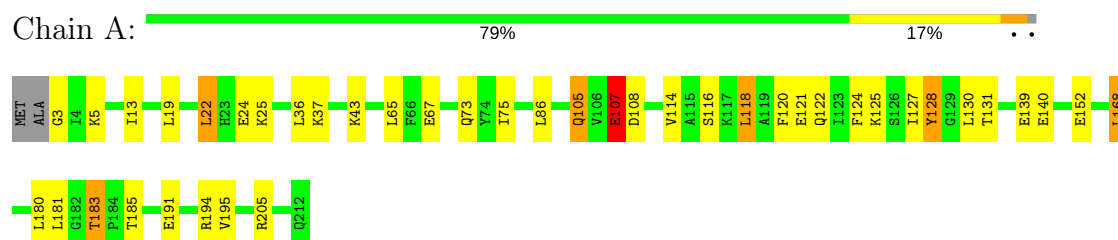
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	V	17	Total	O	0	0
			17	17		
3	W	13	Total	O	0	0
			13	13		
3	X	13	Total	O	0	0
			13	13		



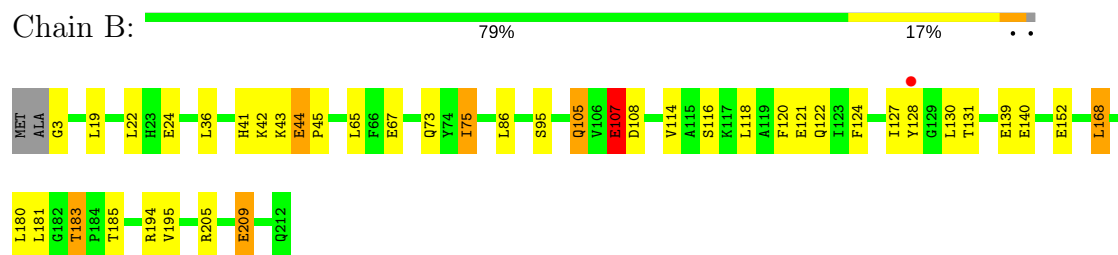
### 3 Residue-property plots [i](#)

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.

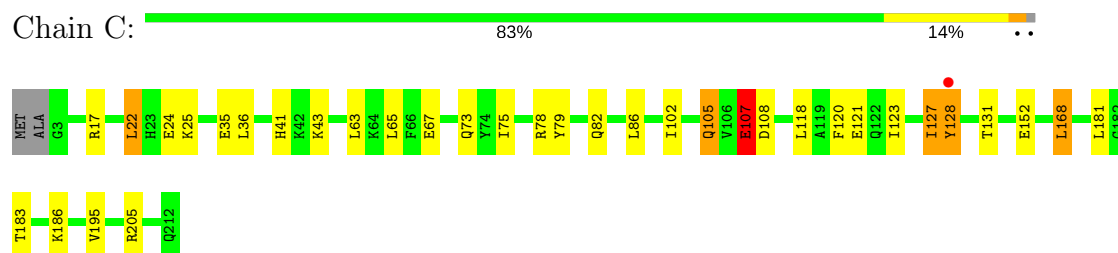
#### • Molecule 1: GLUTATHIONE S-TRANSFERASE F2



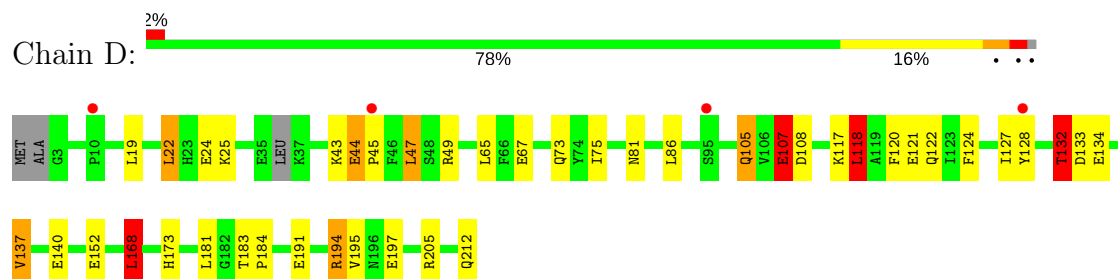
#### • Molecule 1: GLUTATHIONE S-TRANSFERASE F2



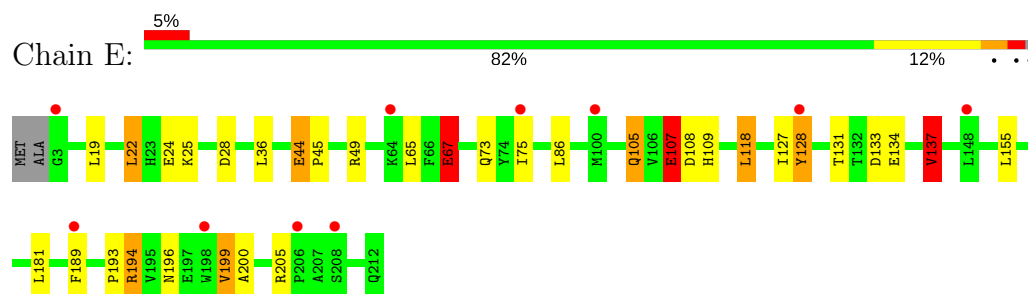
#### • Molecule 1: GLUTATHIONE S-TRANSFERASE F2



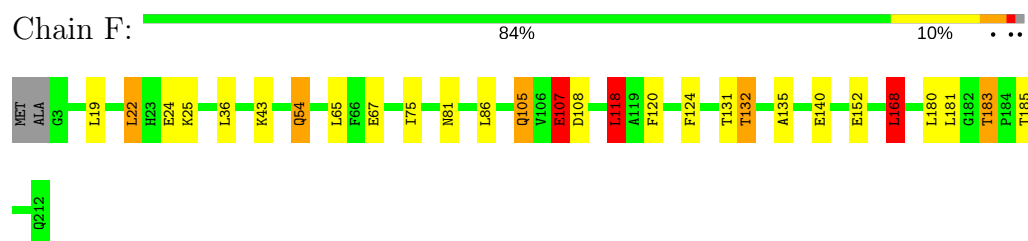
#### • Molecule 1: GLUTATHIONE S-TRANSFERASE F2



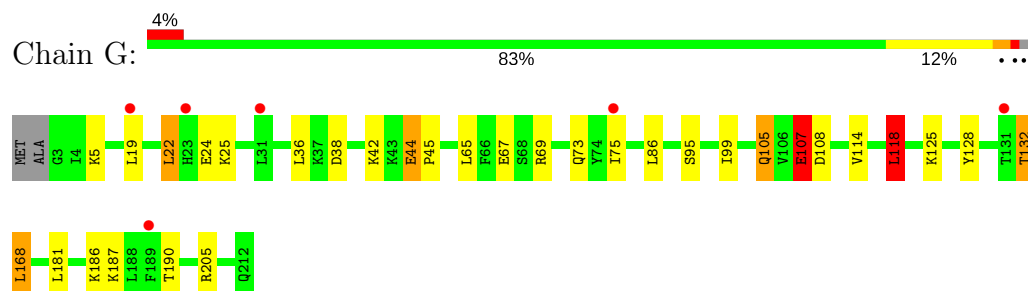
## ● Molecule 1: GLUTATHIONE S-TRANSFERASE F2



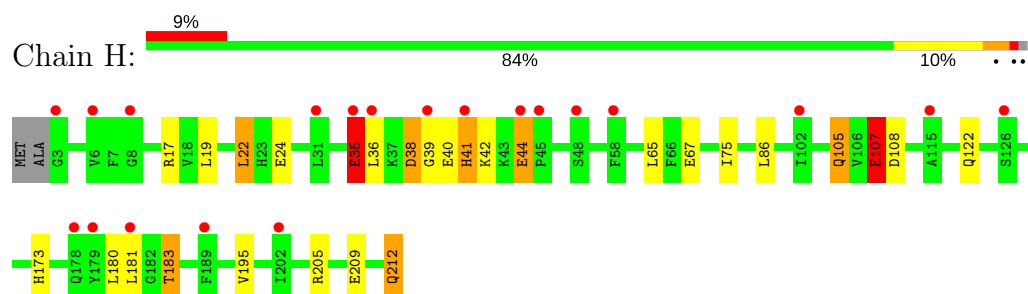
## ● Molecule 1: GLUTATHIONE S-TRANSFERASE F2



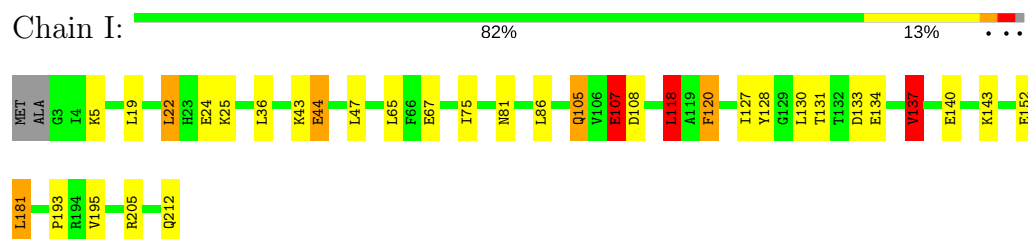
## ● Molecule 1: GLUTATHIONE S-TRANSFERASE F2



## ● Molecule 1: GLUTATHIONE S-TRANSFERASE F2

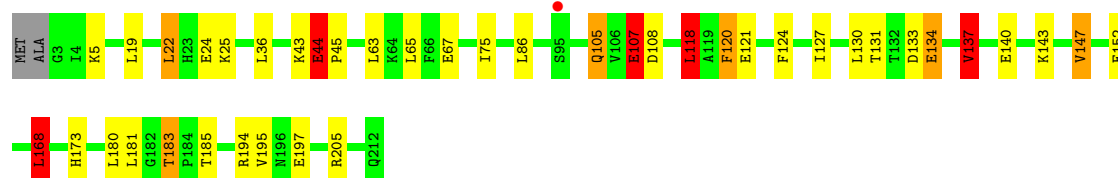


## ● Molecule 1: GLUTATHIONE S-TRANSFERASE F2




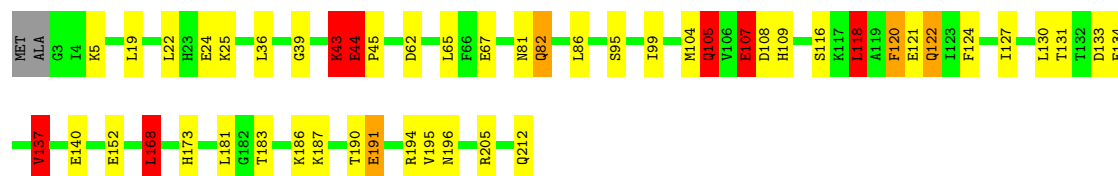
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain J: 




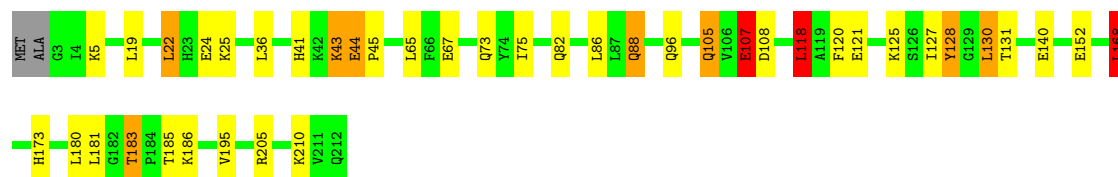
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain K: 




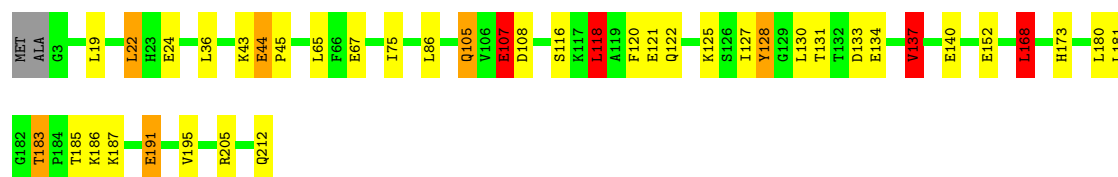
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain L: 




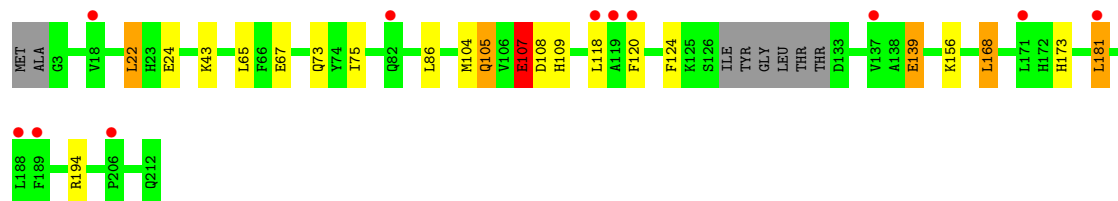
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

Chain M: 

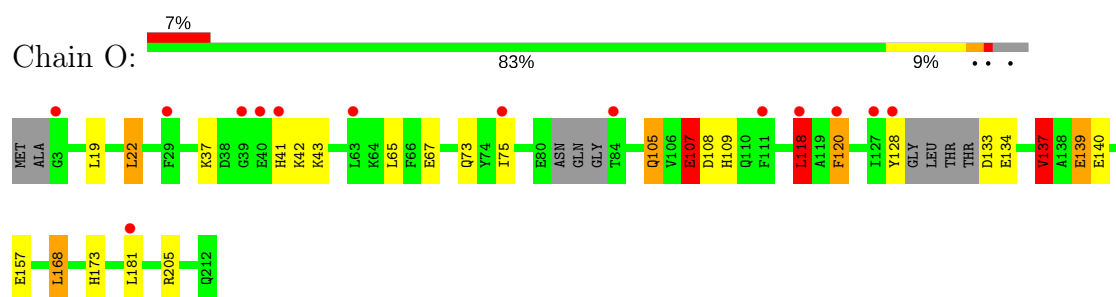


- Molecule 1: GLUTATHIONE S-TRANSFERASE F2

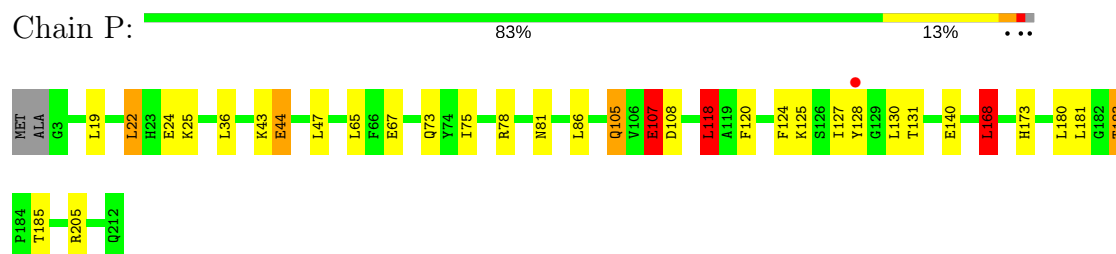
Chain N: 



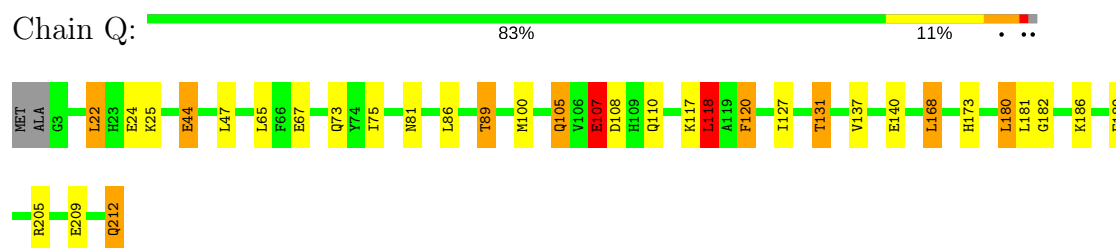
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2



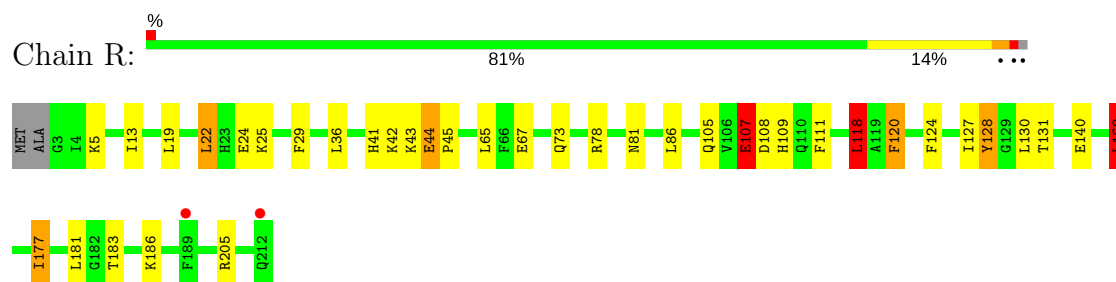
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2



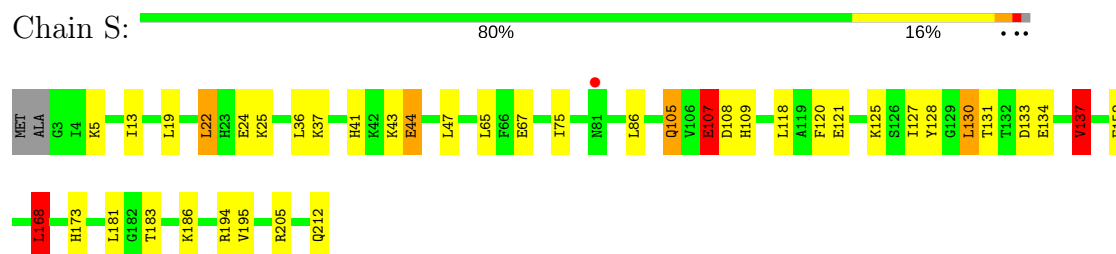
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2



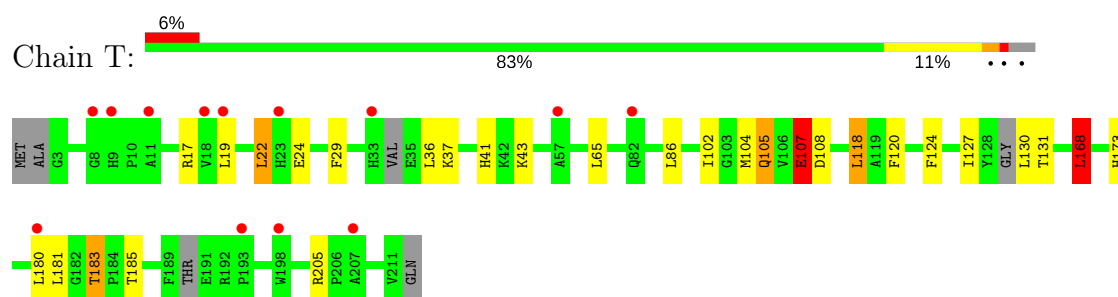
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2



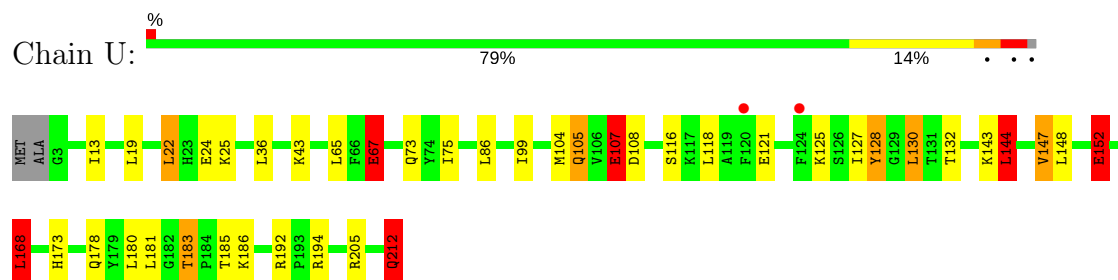
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2



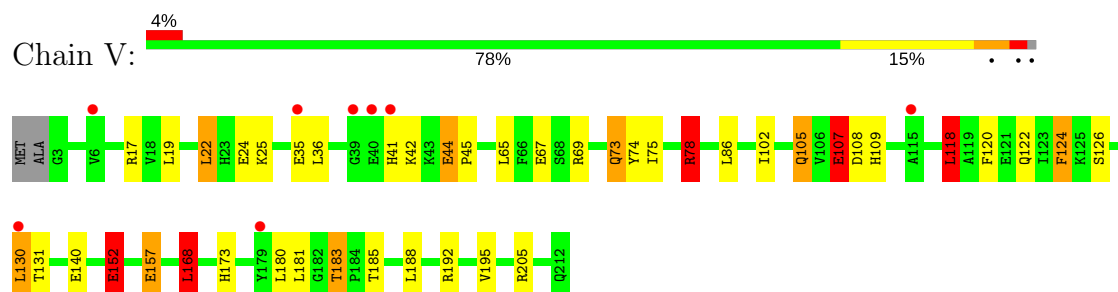
- Molecule 1: GLUTATHIONE S-TRANSFERASE F2



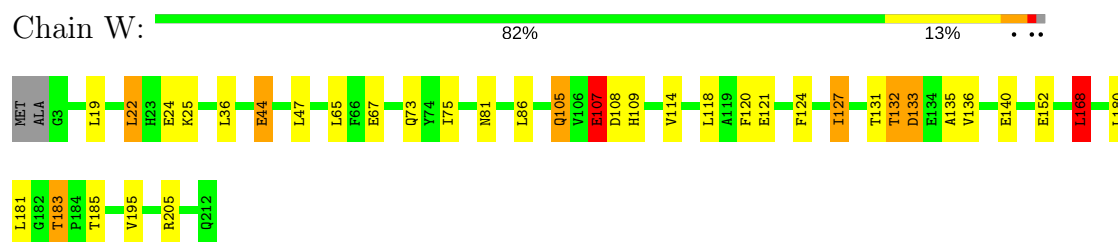
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2



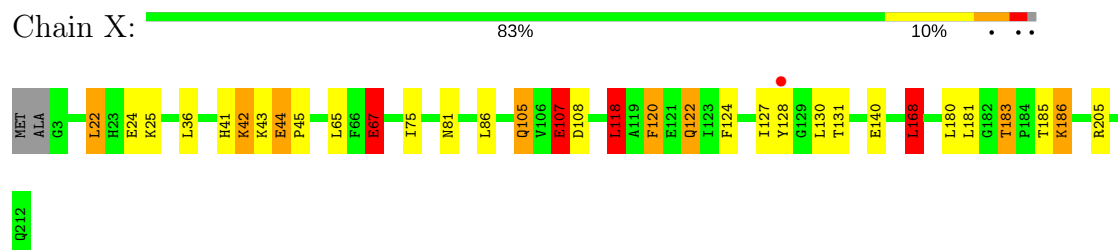
• Molecule 1: GLUTATHIONE S-TRANSFERASE F2



• Molecule 1: GLUTATHIONE S-TRANSFERASE F2



• Molecule 1: GLUTATHIONE S-TRANSFERASE F2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.10Å 113.72Å 132.02Å 83.65° 79.47° 65.85°	Depositor
Resolution (Å)	87.58 – 2.77 87.58 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.6 (87.58-2.77) 97.2 (87.58-2.77)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.250 , 0.284 0.250 , 0.282	Depositor DCC
$R_{free}$ test set	6116 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for -h,-h+k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	39024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8208e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 7WB

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	0.68	2/1639 (0.1%)	0.99	13/2233 (0.6%)
1	B	0.71	2/1691 (0.1%)	1.02	14/2298 (0.6%)
1	C	0.71	2/1647 (0.1%)	0.97	11/2246 (0.5%)
1	D	0.70	2/1624 (0.1%)	1.04	18/2213 (0.8%)
1	E	0.77	6/1590 (0.4%)	1.19	17/2175 (0.8%)
1	F	0.67	2/1645 (0.1%)	0.93	8/2240 (0.4%)
1	G	0.70	2/1581 (0.1%)	1.03	12/2159 (0.6%)
1	H	0.64	2/1547 (0.1%)	0.90	8/2119 (0.4%)
1	I	0.59	0/1681	0.92	5/2284 (0.2%)
1	J	0.66	2/1676 (0.1%)	0.93	9/2275 (0.4%)
1	K	0.69	3/1671 (0.2%)	1.00	16/2270 (0.7%)
1	L	0.64	1/1682 (0.1%)	0.95	7/2284 (0.3%)
1	M	0.63	2/1679 (0.1%)	0.95	10/2281 (0.4%)
1	N	0.59	0/1534	0.88	8/2100 (0.4%)
1	O	0.61	0/1494	1.00	11/2048 (0.5%)
1	P	0.60	0/1652	0.98	8/2252 (0.4%)
1	Q	0.69	2/1655 (0.1%)	1.06	13/2252 (0.6%)
1	R	0.67	2/1662 (0.1%)	0.99	11/2260 (0.5%)
1	S	0.64	1/1690 (0.1%)	1.04	13/2295 (0.6%)
1	T	0.56	0/1503	0.91	12/2057 (0.6%)
1	U	0.74	4/1681 (0.2%)	1.00	15/2282 (0.7%)
1	V	0.75	3/1668 (0.2%)	1.01	15/2267 (0.7%)
1	W	0.72	3/1675 (0.2%)	1.09	10/2277 (0.4%)
1	X	0.70	4/1682 (0.2%)	0.95	8/2284 (0.4%)
All	All	0.67	47/39249 (0.1%)	0.99	272/53451 (0.5%)

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	V	0	1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	107	GLU	CD-OE2	-11.13	1.13	1.25
1	B	107	GLU	CD-OE2	-10.54	1.14	1.25
1	R	107	GLU	CD-OE2	-10.35	1.14	1.25
1	X	107	GLU	CD-OE2	-10.33	1.14	1.25
1	V	152	GLU	CD-OE1	-10.26	1.14	1.25

The worst 5 of 272 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	133	ASP	CB-CG-OD2	18.94	135.35	118.30
1	E	194	ARG	NE-CZ-NH1	15.61	128.10	120.30
1	S	205	ARG	NE-CZ-NH1	15.03	127.81	120.30
1	G	205	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	O	205	ARG	NE-CZ-NH1	14.27	127.44	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	V	152	GLU	Sidechain

## 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	1602	0	1526	38	0
1	B	1650	0	1587	39	0
1	C	1610	0	1528	32	0
1	D	1589	0	1486	35	0
1	E	1553	0	1414	34	0
1	F	1609	0	1546	25	0
1	G	1543	0	1401	23	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1515	0	1343	30	0
1	I	1644	0	1589	41	0
1	J	1640	0	1593	39	0
1	K	1635	0	1580	54	0
1	L	1645	0	1598	41	1
1	M	1642	0	1586	40	0
1	N	1501	0	1371	15	0
1	O	1461	0	1303	32	0
1	P	1615	0	1531	33	0
1	Q	1619	0	1548	31	0
1	R	1625	0	1573	33	1
1	S	1653	0	1604	32	0
1	T	1473	0	1293	23	0
1	U	1644	0	1600	42	0
1	V	1632	0	1569	51	0
1	W	1639	0	1584	26	0
1	X	1645	0	1597	38	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
2	E	14	0	0	0	0
2	F	14	0	0	0	0
2	G	14	0	0	0	0
2	H	14	0	0	0	0
2	I	14	0	0	0	0
2	J	14	0	0	0	0
2	K	14	0	0	0	0
2	L	14	0	0	0	0
2	M	14	0	0	0	0
2	N	14	0	0	0	0
2	O	14	0	0	0	0
2	P	14	0	0	0	0
2	Q	14	0	0	0	0
2	R	14	0	0	0	0
2	S	14	0	0	0	0
2	T	14	0	0	0	0
2	U	14	0	0	0	0
2	V	14	0	0	0	0
2	W	14	0	0	0	0
2	X	14	0	0	0	0
3	A	18	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	1	0
3	C	13	0	0	1	0
3	D	15	0	0	0	0
3	E	19	0	0	2	0
3	F	10	0	0	0	0
3	G	13	0	0	0	0
3	H	6	0	0	0	0
3	I	15	0	0	0	0
3	J	22	0	0	0	0
3	K	13	0	0	1	0
3	L	13	0	0	1	0
3	M	15	0	0	1	0
3	N	9	0	0	0	0
3	O	7	0	0	0	0
3	P	9	0	0	0	0
3	Q	9	0	0	0	0
3	R	3	0	0	0	0
3	S	13	0	0	0	0
3	T	4	0	0	0	0
3	U	20	0	0	1	0
3	V	17	0	0	0	0
3	W	13	0	0	0	0
3	X	13	0	0	1	0
All	All	39024	0	36350	612	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.

The worst 5 of 612 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:H:180:LEU:O	1:H:183:THR:HG22	1.41	1.20
1:E:44:GLU:CB	1:K:190:THR:HG23	1.77	1.15
1:H:36:LEU:HD23	1:H:41:HIS:CG	2.00	0.97
1:D:67:GLU:OE2	1:N:109:HIS:HD2	1.48	0.96
1:Q:180:LEU:HD23	1:Q:189:PHE:HE2	1.30	0.95

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:L:210:LYS:NZ	1:R:81:ASN:OD1[1_556]	1.99	0.21

## 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	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	B	209/212 (99%)	205 (98%)	4 (2%)	0	100	100
1	C	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	D	205/212 (97%)	201 (98%)	4 (2%)	0	100	100
1	E	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	F	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	G	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
1	H	208/212 (98%)	200 (96%)	7 (3%)	1 (0%)	32	65
1	I	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	J	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	K	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	L	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	M	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	N	200/212 (94%)	196 (98%)	4 (2%)	0	100	100
1	O	197/212 (93%)	193 (98%)	4 (2%)	0	100	100
1	P	208/212 (98%)	203 (98%)	5 (2%)	0	100	100
1	Q	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	R	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	S	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	T	198/212 (93%)	194 (98%)	4 (2%)	0	100	100
1	U	208/212 (98%)	204 (98%)	4 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	W	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
1	X	208/212 (98%)	204 (98%)	4 (2%)	0	100	100
All	All	4962/5088 (98%)	4857 (98%)	104 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	41	HIS

### 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	156/182 (86%)	145 (93%)	11 (7%)	17	41
1	B	169/182 (93%)	158 (94%)	11 (6%)	20	47
1	C	159/182 (87%)	152 (96%)	7 (4%)	33	65
1	D	154/182 (85%)	140 (91%)	14 (9%)	11	29
1	E	143/182 (79%)	132 (92%)	11 (8%)	15	37
1	F	160/182 (88%)	147 (92%)	13 (8%)	14	35
1	G	139/182 (76%)	129 (93%)	10 (7%)	17	41
1	H	136/182 (75%)	124 (91%)	12 (9%)	12	31
1	I	168/182 (92%)	152 (90%)	16 (10%)	10	26
1	J	168/182 (92%)	150 (89%)	18 (11%)	8	21
1	K	165/182 (91%)	149 (90%)	16 (10%)	9	25
1	L	169/182 (93%)	152 (90%)	17 (10%)	9	23
1	M	167/182 (92%)	153 (92%)	14 (8%)	13	33
1	N	138/182 (76%)	133 (96%)	5 (4%)	40	73
1	O	128/182 (70%)	120 (94%)	8 (6%)	21	49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	162/182 (89%)	148 (91%)	14 (9%)	12	32
1	Q	162/182 (89%)	152 (94%)	10 (6%)	21	50
1	R	164/182 (90%)	152 (93%)	12 (7%)	16	40
1	S	171/182 (94%)	157 (92%)	14 (8%)	13	34
1	T	129/182 (71%)	120 (93%)	9 (7%)	18	42
1	U	168/182 (92%)	154 (92%)	14 (8%)	13	34
1	V	165/182 (91%)	149 (90%)	16 (10%)	9	25
1	W	168/182 (92%)	154 (92%)	14 (8%)	13	34
1	X	168/182 (92%)	152 (90%)	16 (10%)	10	26
All	All	3776/4368 (86%)	3474 (92%)	302 (8%)	14	36

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	137	VAL
1	M	183	THR
1	W	107	GLU
1	L	19	LEU
1	L	168	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	212	GLN
1	O	41	HIS
1	V	122	GLN
1	N	109	HIS
1	N	122	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

24 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	7WB	A	1213	-	15,16,16	3.34	7 (46%)	13,22,22	2.16	4 (30%)
2	7WB	B	1213	-	15,16,16	3.24	8 (53%)	13,22,22	2.08	4 (30%)
2	7WB	C	1213	-	15,16,16	3.07	8 (53%)	13,22,22	2.01	4 (30%)
2	7WB	D	1213	-	15,16,16	2.71	8 (53%)	13,22,22	2.08	4 (30%)
2	7WB	E	1213	-	15,16,16	3.53	8 (53%)	13,22,22	1.98	4 (30%)
2	7WB	F	1213	-	15,16,16	4.21	8 (53%)	13,22,22	2.15	5 (38%)
2	7WB	G	1213	-	15,16,16	3.49	8 (53%)	13,22,22	1.99	4 (30%)
2	7WB	H	1213	-	15,16,16	2.90	7 (46%)	13,22,22	1.85	4 (30%)
2	7WB	I	1213	-	15,16,16	3.32	8 (53%)	13,22,22	2.36	5 (38%)
2	7WB	J	1213	-	15,16,16	2.78	8 (53%)	13,22,22	2.09	4 (30%)
2	7WB	K	1213	-	15,16,16	3.36	8 (53%)	13,22,22	2.06	4 (30%)
2	7WB	L	1213	-	15,16,16	3.53	8 (53%)	13,22,22	2.09	4 (30%)
2	7WB	M	1213	-	15,16,16	3.06	8 (53%)	13,22,22	2.12	4 (30%)
2	7WB	N	1213	-	15,16,16	3.05	7 (46%)	13,22,22	1.91	4 (30%)
2	7WB	O	1213	-	15,16,16	2.84	8 (53%)	13,22,22	2.11	4 (30%)
2	7WB	P	1213	-	15,16,16	3.53	8 (53%)	13,22,22	2.11	4 (30%)
2	7WB	Q	1213	-	15,16,16	3.49	8 (53%)	13,22,22	1.94	4 (30%)
2	7WB	R	1213	-	15,16,16	3.58	8 (53%)	13,22,22	2.03	4 (30%)
2	7WB	S	1213	-	15,16,16	3.73	8 (53%)	13,22,22	2.17	4 (30%)
2	7WB	T	1212	-	15,16,16	2.74	7 (46%)	13,22,22	2.18	4 (30%)
2	7WB	U	1213	-	15,16,16	3.43	8 (53%)	13,22,22	2.10	4 (30%)
2	7WB	V	1213	-	15,16,16	2.82	7 (46%)	13,22,22	1.92	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	7WB	W	1213	-	15,16,16	3.84	8 (53%)	13,22,22	2.21	4 (30%)
2	7WB	X	1213	-	15,16,16	3.14	8 (53%)	13,22,22	2.10	4 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7WB	A	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	B	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	C	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	D	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	E	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	F	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	G	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	H	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	I	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	J	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	K	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	L	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	M	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	N	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	O	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	P	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	Q	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	R	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	S	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	T	1212	-	-	0/0/13/13	0/3/3/3
2	7WB	U	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	V	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	W	1213	-	-	0/0/13/13	0/3/3/3
2	7WB	X	1213	-	-	0/0/13/13	0/3/3/3

The worst 5 of 187 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1213	7WB	CAK-SAJ	-12.37	1.54	1.74
2	S	1213	7WB	CAK-SAJ	-10.06	1.57	1.74
2	E	1213	7WB	CAK-SAJ	-9.39	1.59	1.74
2	W	1213	7WB	CAK-SAJ	-8.73	1.60	1.74
2	A	1213	7WB	CAK-SAJ	-8.49	1.60	1.74

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	1213	7WB	CAN-CAM-NAI	-5.48	107.20	112.90
2	W	1213	7WB	CAN-CAM-NAI	-5.16	107.52	112.90
2	I	1213	7WB	CAN-CAM-NAI	-5.10	107.58	112.90
2	B	1213	7WB	CAN-CAM-NAI	-5.05	107.64	112.90
2	X	1213	7WB	CAN-CAM-NAI	-5.04	107.66	112.90

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	210/212 (99%)	-0.11	0 100 100	26, 43, 58, 71	0
1	B	210/212 (99%)	-0.13	1 (0%) 90 89	25, 42, 61, 75	0
1	C	210/212 (99%)	-0.12	1 (0%) 90 89	30, 48, 68, 87	0
1	D	209/212 (98%)	0.12	4 (1%) 67 62	33, 49, 72, 102	0
1	E	210/212 (99%)	0.38	11 (5%) 28 21	42, 60, 76, 84	0
1	F	210/212 (99%)	-0.17	0 100 100	24, 43, 69, 84	0
1	G	210/212 (99%)	0.31	8 (3%) 41 34	37, 62, 84, 96	0
1	H	210/212 (99%)	0.59	20 (9%) 9 5	43, 67, 103, 141	0
1	I	210/212 (99%)	-0.17	0 100 100	20, 41, 59, 77	0
1	J	210/212 (99%)	-0.14	1 (0%) 90 89	23, 38, 51, 68	0
1	K	210/212 (99%)	-0.15	0 100 100	27, 41, 60, 71	0
1	L	210/212 (99%)	-0.19	0 100 100	21, 37, 55, 69	0
1	M	210/212 (99%)	-0.23	0 100 100	21, 36, 53, 68	0
1	N	204/212 (96%)	0.37	11 (5%) 26 20	39, 62, 83, 91	0
1	O	203/212 (95%)	0.48	14 (6%) 18 12	43, 68, 90, 110	0
1	P	210/212 (99%)	-0.01	1 (0%) 90 89	27, 48, 71, 92	0
1	Q	210/212 (99%)	-0.03	0 100 100	26, 48, 68, 85	0
1	R	210/212 (99%)	-0.09	2 (0%) 82 79	27, 48, 70, 81	0
1	S	210/212 (99%)	-0.26	1 (0%) 90 89	20, 37, 53, 67	0
1	T	206/212 (97%)	0.42	13 (6%) 21 15	36, 70, 90, 103	0
1	U	210/212 (99%)	-0.09	2 (0%) 82 79	24, 42, 61, 71	0
1	V	210/212 (99%)	0.16	8 (3%) 41 34	26, 49, 74, 87	0
1	W	210/212 (99%)	-0.14	0 100 100	23, 39, 61, 85	0
1	X	210/212 (99%)	-0.19	1 (0%) 90 89	21, 38, 55, 68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5022/5088 (98%)	0.02	99 (1%) 65 60	20, 47, 77, 141	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	57	ALA	4.9
1	O	41	HIS	4.5
1	G	19	LEU	4.3
1	R	189	PHE	4.3
1	E	3	GLY	4.1

## 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	7WB	T	1212	14/14	0.90	0.29	3.13	49,54,71,71	0
2	7WB	N	1213	14/14	0.83	0.28	1.62	80,87,93,94	0
2	7WB	A	1213	14/14	0.94	0.18	1.56	34,37,45,48	0
2	7WB	K	1213	14/14	0.93	0.21	1.18	48,55,61,66	0
2	7WB	I	1213	14/14	0.92	0.19	1.15	35,41,60,62	0
2	7WB	R	1213	14/14	0.91	0.26	1.14	62,72,84,85	0
2	7WB	W	1213	14/14	0.95	0.17	1.10	31,35,43,52	0
2	7WB	O	1213	14/14	0.86	0.29	0.71	62,71,88,94	0
2	7WB	C	1213	14/14	0.91	0.17	0.58	38,46,57,62	0
2	7WB	B	1213	14/14	0.94	0.17	0.50	38,42,49,58	0
2	7WB	P	1213	14/14	0.94	0.19	0.40	35,42,56,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	7WB	D	1213	14/14	0.92	0.24	0.39	46,50,51,57	0
2	7WB	X	1213	14/14	0.94	0.18	0.26	39,44,51,56	0
2	7WB	S	1213	14/14	0.92	0.18	0.25	42,48,58,69	0
2	7WB	H	1213	14/14	0.93	0.22	0.25	63,67,74,78	0
2	7WB	L	1213	14/14	0.94	0.18	0.19	38,40,43,46	0
2	7WB	G	1213	14/14	0.91	0.21	0.18	54,57,64,69	0
2	7WB	Q	1213	14/14	0.94	0.19	0.15	49,54,58,61	0
2	7WB	M	1213	14/14	0.95	0.17	0.15	35,38,41,42	0
2	7WB	E	1213	14/14	0.87	0.20	0.05	50,59,68,72	0
2	7WB	V	1213	14/14	0.94	0.16	-0.11	46,48,61,66	0
2	7WB	F	1213	14/14	0.96	0.18	-0.17	38,42,50,55	0
2	7WB	U	1213	14/14	0.96	0.14	-0.99	33,37,52,60	0
2	7WB	J	1213	14/14	0.95	0.14	-1.25	33,40,46,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.