



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 1, 2025 – 11:37 pm BST

PDB ID : 2J58 / pdb\_00002j58  
Title : The structure of Wza  
Authors : Dong, C.; Naismith, J.H.  
Deposited on : 2006-09-12  
Resolution : 2.25 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)

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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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

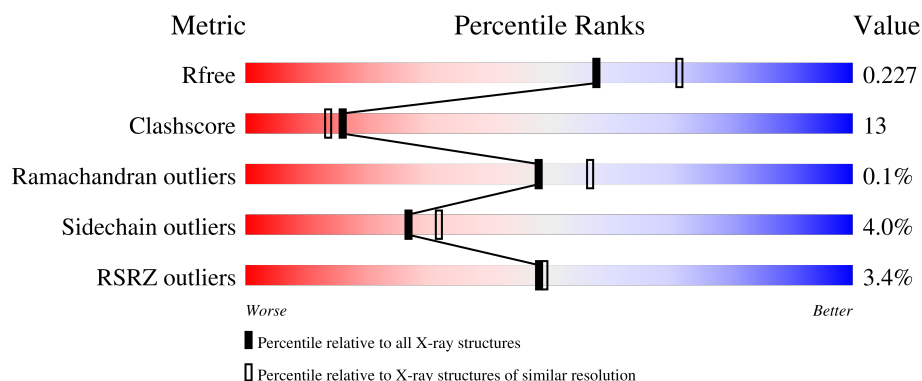
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



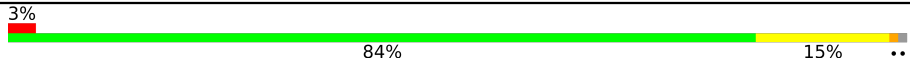


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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  $\geq 3$ , 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	359	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	359	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	C	359	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
1	D	359	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	E	359	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	359	
1	G	359	
1	H	359	

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
1	SC2	D	21	-	-	X	-
1	SC2	E	21	-	-	X	-

## 2 Entry composition

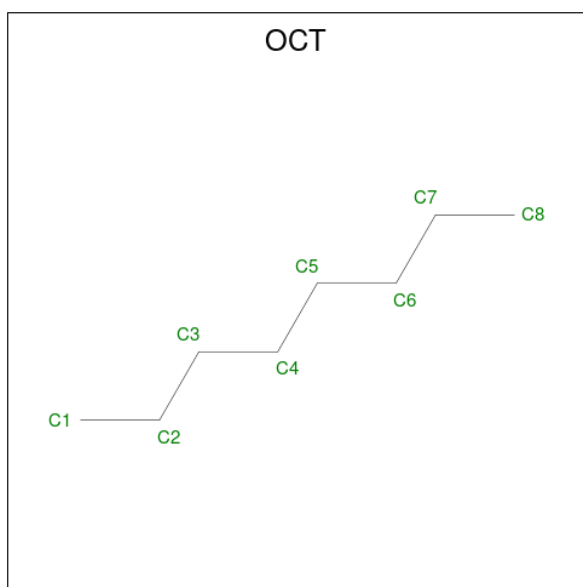
There are 5 unique types of molecules in this entry. The entry contains 23866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OUTER MEMBRANE LIPOPROTEIN WZA.

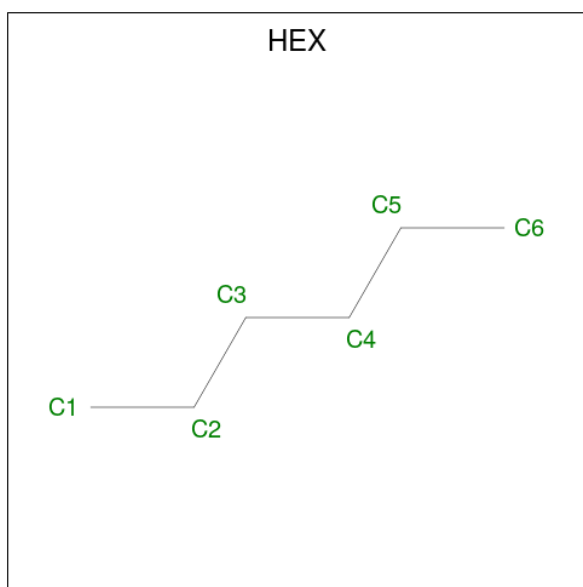
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	B	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	C	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	D	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	E	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	F	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	G	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			
1	H	356	Total	C	N	O	S	Se	0	0	0
			2755	1737	471	536	1	10			

- Molecule 2 is N-OCTANE (CCD ID: OCT) (formula: C<sub>8</sub>H<sub>18</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0
2	D	1	Total C 8 8	0	0
2	E	1	Total C 8 8	0	0
2	F	1	Total C 8 8	0	0
2	G	1	Total C 8 8	0	0
2	H	1	Total C 8 8	0	0

- Molecule 3 is HEXANE (CCD ID: HEX) (formula: C<sub>6</sub>H<sub>14</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	C	1	Total C 6 6	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 6 6	0	0
3	F	1	Total C 6 6	0	0
3	G	1	Total C 6 6	0	0
3	H	1	Total C 6 6	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

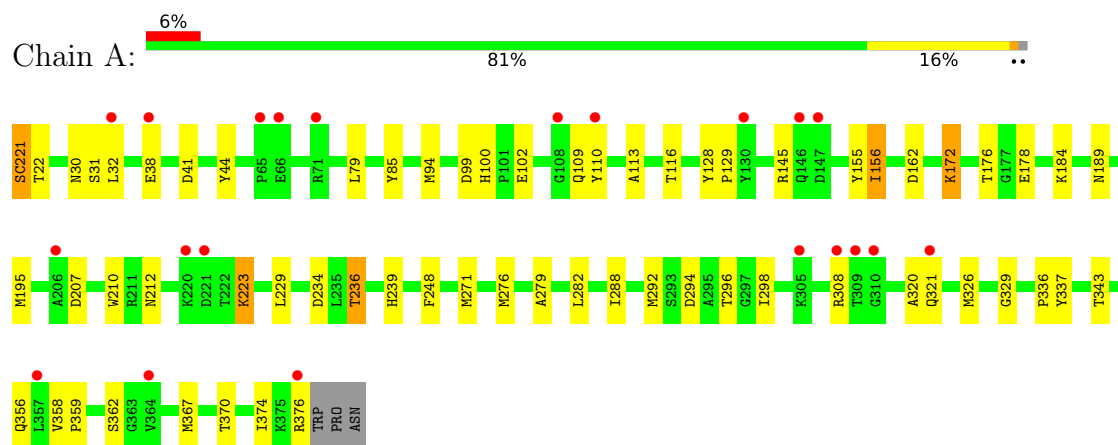
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	167	Total	O		0	0
			167	167			
5	B	199	Total	O		0	0
			199	199			
5	C	229	Total	O		0	0
			229	229			
5	D	157	Total	O		0	0
			157	157			
5	E	191	Total	O		0	0
			191	191			
5	F	231	Total	O		0	0
			231	231			
5	G	227	Total	O		0	0
			227	227			
5	H	233	Total	O		0	0
			233	233			



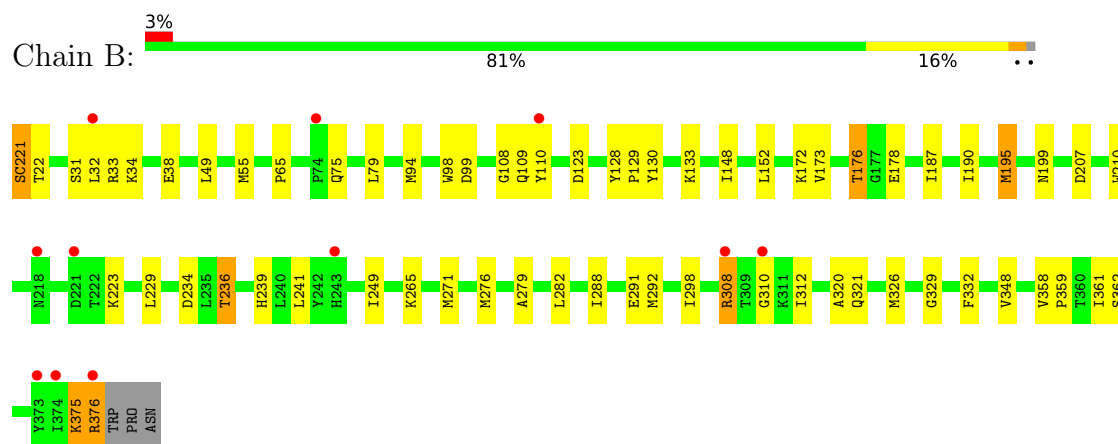
### 3 Residue-property plots [i](#)

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.

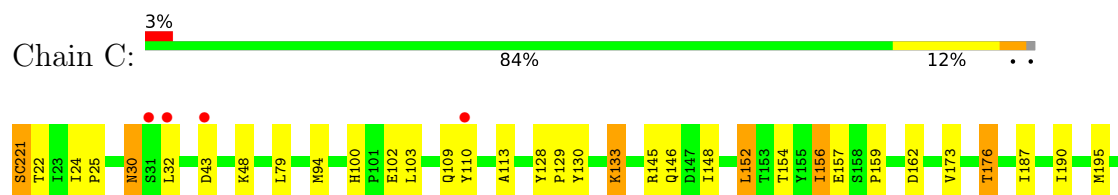
#### • Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

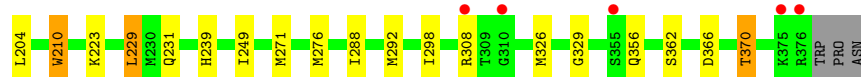


#### • Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

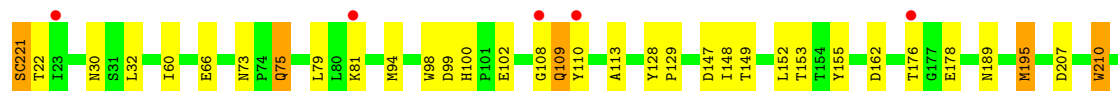
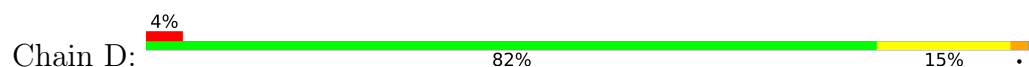


#### • Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

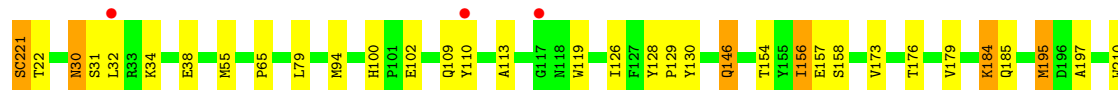
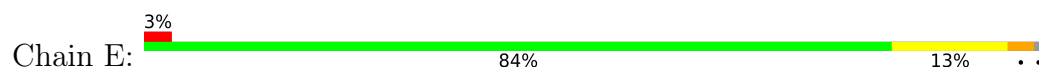




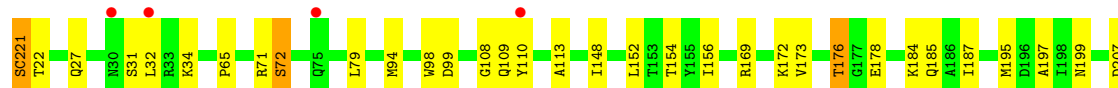
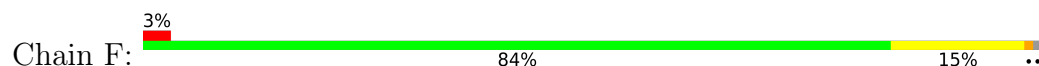
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA



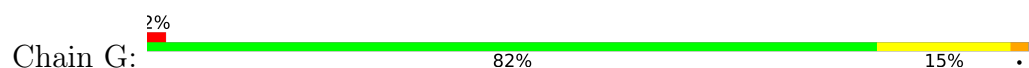
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA



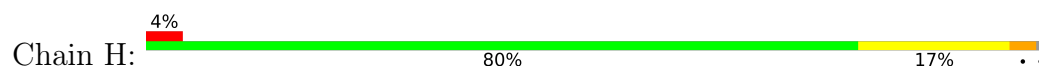
• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA

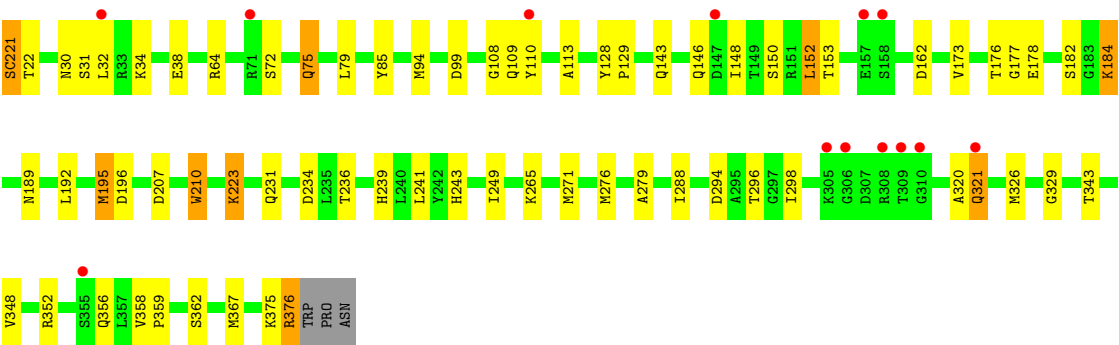


• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA



• Molecule 1: OUTER MEMBRANE LIPOPROTEIN WZA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.72Å 215.27Å 220.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.83 – 2.25 107.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (107.83-2.25) 99.1 (107.83-2.25)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.226 0.190 , 0.227	Depositor DCC
$R_{free}$ test set	10587 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	23866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SC2, SO4, OCT, HEX

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	0.58	4/2785 (0.1%)	0.64	0/3775
1	B	0.56	0/2785	0.65	0/3775
1	C	0.60	0/2785	0.69	0/3775
1	D	0.61	3/2785 (0.1%)	0.65	0/3775
1	E	0.54	0/2785	0.64	0/3775
1	F	0.59	0/2785	0.64	0/3775
1	G	0.58	1/2785 (0.0%)	0.65	0/3775
1	H	0.58	0/2785	0.66	0/3775
All	All	0.58	8/22280 (0.0%)	0.65	0/30200

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	155	TYR	CE2-CZ	11.73	1.53	1.38
1	D	155	TYR	CG-CD2	8.22	1.49	1.39
1	A	155	TYR	CG-CD1	8.19	1.49	1.39
1	D	155	TYR	CG-CD1	7.61	1.49	1.39
1	A	155	TYR	CE2-CZ	7.47	1.48	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2755	0	2762	87	0
1	B	2755	0	2762	86	0
1	C	2755	0	2762	76	0
1	D	2755	0	2762	87	0
1	E	2755	0	2762	94	0
1	F	2755	0	2762	93	0
1	G	2755	0	2762	92	0
1	H	2755	0	2762	94	0
2	A	8	0	18	0	0
2	B	8	0	18	1	0
2	C	8	0	18	0	0
2	D	8	0	18	0	0
2	E	8	0	18	0	0
2	F	8	0	18	0	0
2	G	8	0	18	1	0
2	H	8	0	18	0	0
3	A	6	0	14	0	0
3	B	6	0	14	0	0
3	C	6	0	14	0	0
3	D	6	0	14	0	0
3	E	6	0	14	0	0
3	F	6	0	14	0	0
3	G	6	0	14	0	0
3	H	6	0	14	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	10	0	0	0	0
5	A	167	0	0	12	0
5	B	199	0	0	11	0
5	C	229	0	0	13	0
5	D	157	0	0	12	0
5	E	191	0	0	10	0
5	F	231	0	0	20	0
5	G	227	0	0	16	0
5	H	233	0	0	21	0
All	All	23866	0	22352	577	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 13.

The worst 5 of 577 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:C:326:MSE:CE	1:C:329:GLY:HA3	1.28	1.60
1:A:110:TYR:CZ	1:D:110:TYR:CE1	1.95	1.53
1:E:110:TYR:CZ	1:F:110:TYR:CE1	1.93	1.52
1:B:110:TYR:CE1	1:G:110:TYR:CZ	1.97	1.51
1:B:326:MSE:CE	1:B:329:GLY:HA3	1.41	1.50

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	353/359 (98%)	344 (98%)	9 (2%)	0	100	100
1	B	353/359 (98%)	345 (98%)	7 (2%)	1 (0%)	37	41
1	C	353/359 (98%)	346 (98%)	7 (2%)	0	100	100
1	D	353/359 (98%)	348 (99%)	5 (1%)	0	100	100
1	E	353/359 (98%)	346 (98%)	7 (2%)	0	100	100
1	F	353/359 (98%)	348 (99%)	5 (1%)	0	100	100
1	G	353/359 (98%)	346 (98%)	6 (2%)	1 (0%)	37	41
1	H	353/359 (98%)	350 (99%)	3 (1%)	0	100	100
All	All	2824/2872 (98%)	2773 (98%)	49 (2%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	LYS
1	G	375	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/297 (102%)	295 (97%)	9 (3%)	36	44
1	B	304/297 (102%)	292 (96%)	12 (4%)	27	33
1	C	304/297 (102%)	290 (95%)	14 (5%)	23	25
1	D	304/297 (102%)	288 (95%)	16 (5%)	19	19
1	E	304/297 (102%)	289 (95%)	15 (5%)	21	23
1	F	304/297 (102%)	296 (97%)	8 (3%)	41	50
1	G	304/297 (102%)	292 (96%)	12 (4%)	27	33
1	H	304/297 (102%)	292 (96%)	12 (4%)	27	33
All	All	2432/2376 (102%)	2334 (96%)	98 (4%)	27	32

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	157	GLU
1	F	210	TRP
1	E	184	LYS
1	E	362	SER
1	G	32	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	118	ASN
1	F	118	ASN
1	H	356	GLN
1	H	218	ASN
1	E	121	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
1	SC2	E	21	1	7,8,9	0.93	0	9,9,11	1.37	1 (11%)
1	SC2	A	21	-	7,8,9	0.80	0	9,9,11	1.28	1 (11%)
1	SC2	C	21	-	7,8,9	1.06	1 (14%)	9,9,11	1.66	4 (44%)
1	SC2	B	21	1	7,8,9	1.02	0	9,9,11	1.36	1 (11%)
1	SC2	G	21	1	7,8,9	1.06	0	9,9,11	1.14	1 (11%)
1	SC2	D	21	1	7,8,9	1.04	1 (14%)	9,9,11	0.91	0
1	SC2	H	21	-	7,8,9	0.97	0	9,9,11	2.11	3 (33%)
1	SC2	F	21	-	7,8,9	0.88	0	9,9,11	1.80	1 (11%)

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
1	SC2	E	21	1	-	0/7/8/10	-
1	SC2	A	21	-	-	2/7/8/10	-
1	SC2	C	21	-	-	3/7/8/10	-
1	SC2	B	21	1	-	4/7/8/10	-
1	SC2	G	21	1	-	3/7/8/10	-
1	SC2	D	21	1	-	2/7/8/10	-
1	SC2	H	21	-	-	3/7/8/10	-
1	SC2	F	21	-	-	3/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	SC2	CM-CT	2.31	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	21	SC2	CM-CT	2.12	1.54	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	21	SC2	CA-CB-SG	-4.19	109.49	114.19
1	H	21	SC2	CB-CA-N	-3.49	106.31	111.28
1	A	21	SC2	CA-CB-SG	-2.71	111.15	114.19
1	E	21	SC2	CB-CA-N	-2.71	107.43	111.28
1	C	21	SC2	CA-CB-SG	-2.60	111.27	114.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	21	SC2	C-CA-CB-SG
1	A	21	SC2	N-CA-CB-SG
1	B	21	SC2	O-C-CA-CB
1	B	21	SC2	C-CA-CB-SG
1	B	21	SC2	N-CA-CB-SG

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	21	SC2	4	0
1	A	21	SC2	2	0
1	C	21	SC2	3	0
1	B	21	SC2	1	0
1	G	21	SC2	2	0
1	D	21	SC2	5	0
1	H	21	SC2	3	0
1	F	21	SC2	3	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

32 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	$\# Z  > 2$
4	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.19	0
4	SO4	C	605	-	4,4,4	0.14	0	6,6,6	0.11	0
3	HEX	D	601	-	5,5,5	0.50	0	4,4,4	0.24	0
3	HEX	F	601	-	5,5,5	0.38	0	4,4,4	0.37	0
2	OCT	B	600	-	7,7,7	0.59	0	6,6,6	0.33	0
3	HEX	G	601	-	5,5,5	0.52	0	4,4,4	0.28	0
4	SO4	H	602	-	4,4,4	0.14	0	6,6,6	0.25	0
4	SO4	H	605	-	4,4,4	0.14	0	6,6,6	0.23	0
4	SO4	F	605	-	4,4,4	0.12	0	6,6,6	0.18	0
4	SO4	G	605	-	4,4,4	0.17	0	6,6,6	0.14	0
2	OCT	E	600	-	7,7,7	0.56	0	6,6,6	0.31	0
2	OCT	H	600	-	7,7,7	0.55	0	6,6,6	0.30	0
4	SO4	A	602	-	4,4,4	0.22	0	6,6,6	0.44	0
3	HEX	A	601	-	5,5,5	0.49	0	4,4,4	0.39	0
4	SO4	A	605	-	4,4,4	0.14	0	6,6,6	0.20	0
4	SO4	C	602	-	4,4,4	0.22	0	6,6,6	0.27	0
3	HEX	C	601	-	5,5,5	0.54	0	4,4,4	0.27	0
4	SO4	D	602	-	4,4,4	0.16	0	6,6,6	0.33	0
2	OCT	F	600	-	7,7,7	0.49	0	6,6,6	0.36	0
2	OCT	D	600	-	7,7,7	0.47	0	6,6,6	0.38	0
4	SO4	F	602	-	4,4,4	0.21	0	6,6,6	0.37	0
3	HEX	B	601	-	5,5,5	0.44	0	4,4,4	0.32	0
4	SO4	E	605	-	4,4,4	0.13	0	6,6,6	0.16	0
4	SO4	G	602	-	4,4,4	0.15	0	6,6,6	0.44	0
4	SO4	D	605	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SO4	E	602	-	4,4,4	0.19	0	6,6,6	0.41	0
3	HEX	E	601	-	5,5,5	0.42	0	4,4,4	0.27	0
2	OCT	G	600	-	7,7,7	0.57	0	6,6,6	0.30	0
3	HEX	H	601	-	5,5,5	0.48	0	4,4,4	0.27	0
2	OCT	A	600	-	7,7,7	0.54	0	6,6,6	0.36	0
4	SO4	B	602	-	4,4,4	0.17	0	6,6,6	0.42	0
2	OCT	C	600	-	7,7,7	0.58	0	6,6,6	0.27	0

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	OCT	E	600	-	-	2/5/5/5	-
2	OCT	H	600	-	-	2/5/5/5	-
3	HEX	A	601	-	-	0/3/3/3	-
3	HEX	D	601	-	-	0/3/3/3	-
3	HEX	C	601	-	-	0/3/3/3	-
2	OCT	F	600	-	-	3/5/5/5	-
2	OCT	D	600	-	-	3/5/5/5	-
3	HEX	F	601	-	-	0/3/3/3	-
3	HEX	E	601	-	-	1/3/3/3	-
2	OCT	B	600	-	-	2/5/5/5	-
2	OCT	G	600	-	-	2/5/5/5	-
3	HEX	G	601	-	-	2/3/3/3	-
3	HEX	B	601	-	-	0/3/3/3	-
3	HEX	H	601	-	-	0/3/3/3	-
2	OCT	A	600	-	-	2/5/5/5	-
2	OCT	C	600	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	600	OCT	C2-C3-C4-C5
2	G	600	OCT	C3-C4-C5-C6
2	C	600	OCT	C2-C3-C4-C5
3	E	601	HEX	C2-C3-C4-C5
2	B	600	OCT	C3-C4-C5-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	OCT	1	0
2	G	600	OCT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1
1	A	1
1	C	1
1	H	1
1	G	1
1	B	1
1	E	1
1	D	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	21:SC2	C	22:THR	N	2.68
1	A	21:SC2	C	22:THR	N	2.55
1	C	21:SC2	C	22:THR	N	2.45
1	H	21:SC2	C	22:THR	N	2.36
1	G	21:SC2	C	22:THR	N	2.35

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	345/359 (96%)	0.65	21 (6%) 28 28	16, 34, 45, 57	1 (0%)
1	B	345/359 (96%)	0.41	11 (3%) 50 51	15, 34, 44, 58	1 (0%)
1	C	345/359 (96%)	0.30	9 (2%) 57 58	16, 34, 43, 58	1 (0%)
1	D	345/359 (96%)	0.53	13 (3%) 44 45	15, 34, 42, 57	1 (0%)
1	E	345/359 (96%)	0.27	10 (2%) 54 54	16, 34, 45, 57	1 (0%)
1	F	345/359 (96%)	0.21	9 (2%) 57 58	16, 34, 45, 58	1 (0%)
1	G	345/359 (96%)	0.14	7 (2%) 64 64	16, 34, 44, 58	1 (0%)
1	H	345/359 (96%)	0.33	13 (3%) 44 45	16, 34, 43, 57	1 (0%)
All	All	2760/2872 (96%)	0.36	93 (3%) 48 49	15, 34, 45, 58	8 (0%)

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	110	TYR	11.6
1	A	110	TYR	11.3
1	E	110	TYR	11.1
1	B	110	TYR	9.7
1	F	110	TYR	9.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	SC2	C	21	9/10	0.64	0.27	73,74,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SC2	H	21	9/10	0.72	0.24	67,68,68,69	0
1	SC2	D	21	9/10	0.73	0.29	70,71,71,71	0
1	SC2	B	21	9/10	0.74	0.26	69,70,71,71	0
1	SC2	G	21	9/10	0.75	0.24	72,74,75,75	0
1	SC2	F	21	9/10	0.79	0.23	77,78,78,78	0
1	SC2	A	21	9/10	0.83	0.20	75,76,76,78	0
1	SC2	E	21	9/10	0.88	0.16	57,59,59,61	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	H	605	5/5	0.60	0.23	111,111,111,111	0
4	SO4	B	605	5/5	0.66	0.19	122,122,122,122	0
4	SO4	F	605	5/5	0.70	0.20	99,99,99,100	0
3	HEX	H	601	6/6	0.73	0.24	50,51,51,51	0
3	HEX	G	601	6/6	0.73	0.24	43,44,46,46	0
2	OCT	H	600	8/8	0.74	0.28	55,57,59,59	0
2	OCT	C	600	8/8	0.74	0.23	44,46,47,48	0
4	SO4	D	605	5/5	0.75	0.17	114,114,115,115	0
4	SO4	A	605	5/5	0.75	0.16	92,93,93,94	0
3	HEX	C	601	6/6	0.75	0.20	43,43,44,44	0
4	SO4	G	605	5/5	0.76	0.17	98,99,99,99	0
2	OCT	E	600	8/8	0.77	0.25	52,52,53,54	0
4	SO4	C	605	5/5	0.77	0.17	100,100,101,101	0
2	OCT	G	600	8/8	0.78	0.28	50,58,62,62	0
3	HEX	D	601	6/6	0.79	0.20	46,46,47,48	0
2	OCT	B	600	8/8	0.79	0.26	53,54,58,58	0
4	SO4	E	605	5/5	0.80	0.15	96,96,96,97	0
3	HEX	B	601	6/6	0.80	0.22	46,48,49,50	0
2	OCT	D	600	8/8	0.80	0.27	55,56,58,59	0
2	OCT	A	600	8/8	0.80	0.23	48,54,55,55	0
2	OCT	F	600	8/8	0.83	0.23	55,56,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEX	E	601	6/6	0.84	0.25	50,50,52,53	0
3	HEX	A	601	6/6	0.85	0.15	39,40,42,42	0
3	HEX	F	601	6/6	0.85	0.20	48,48,49,51	0
4	SO4	A	602	5/5	0.96	0.16	48,50,51,51	0
4	SO4	H	602	5/5	0.97	0.14	41,42,43,45	0
4	SO4	B	602	5/5	0.97	0.12	52,52,53,53	0
4	SO4	C	602	5/5	0.98	0.14	35,35,37,37	0
4	SO4	G	602	5/5	0.98	0.13	42,43,43,45	0
4	SO4	E	602	5/5	0.98	0.12	37,42,44,45	0
4	SO4	D	602	5/5	0.98	0.14	49,50,53,53	0
4	SO4	F	602	5/5	0.98	0.13	37,37,40,41	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.