



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2026 – 12:13 PM EDT

PDB ID : 9PS9 / pdb\_00009ps9  
Title : High-resolution crystal structure of Vibrio cholerae NFeoB in the apo form in orthorhombic space group  
Authors : Magante, K.; Lee, M.; Smith, A.T.  
Deposited on : 2025-07-25  
Resolution : 1.85 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

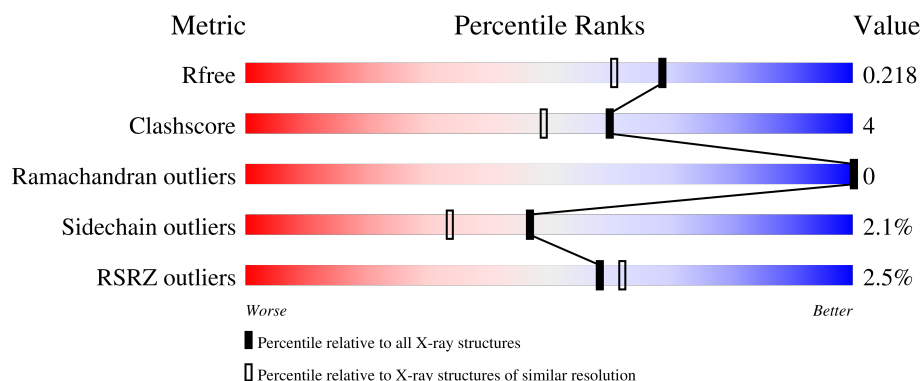
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

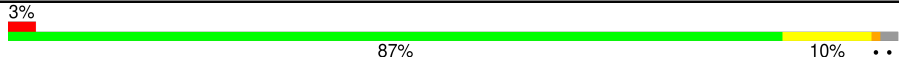

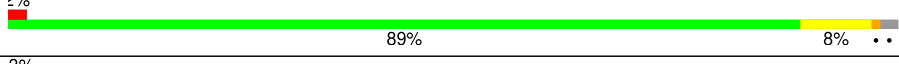

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	261	
1	B	261	
1	C	261	
1	D	261	

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
3	ETF	A	306	-	-	X	-
3	ETF	B	303	-	-	X	-
3	ETF	B	306	-	-	X	-
3	ETF	C	302	-	-	X	-
3	ETF	C	305	-	-	X	-
3	ETF	D	304	-	-	X	-
3	ETF	D	305	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9174 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 Ferrous iron transport protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2034	1278	367	381	8			
1	B	256	Total	C	N	O	S	0	0	0
			2028	1275	366	379	8			
1	C	256	Total	C	N	O	S	0	0	0
			2028	1275	366	379	8			
1	D	256	Total	C	N	O	S	0	0	0
			2028	1275	366	379	8			

There are 4 discrepancies between the modelled and reference sequences:

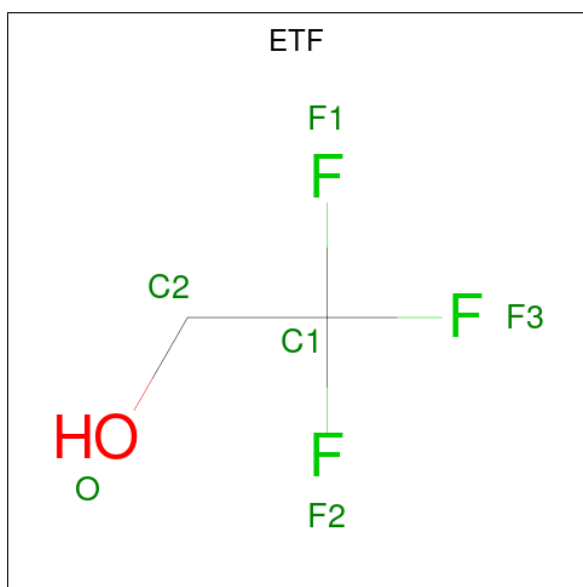
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP A0A655NVH2
B	1	SER	-	expression tag	UNP A0A655NVH2
C	1	SER	-	expression tag	UNP A0A655NVH2
D	1	SER	-	expression tag	UNP A0A655NVH2

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is TRIFLUOROETHANOL (CCD ID: ETF) (formula:  $C_2H_3F_3O$ ).



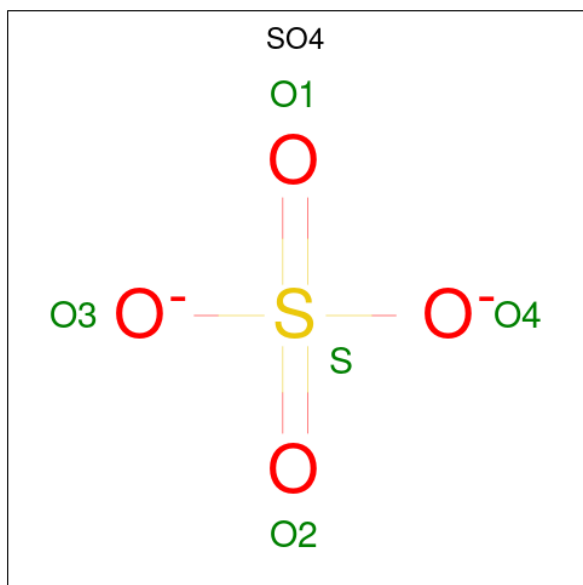
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			6	2	3	1		
3	A	1	Total	C	F	O	0	0
			6	2	3	1		
3	A	1	Total	C	F	O	0	0
			6	2	3	1		
3	A	1	Total	C	F	O	0	0
			6	2	3	1		
3	B	1	Total	C	F	O	0	0
			6	2	3	1		
3	B	1	Total	C	F	O	0	0
			6	2	3	1		
3	B	1	Total	C	F	O	0	0
			6	2	3	1		
3	B	1	Total	C	F	O	0	0
			6	2	3	1		
3	B	1	Total	C	F	O	0	0
			6	2	3	1		
3	C	1	Total	C	F	O	0	0
			6	2	3	1		
3	C	1	Total	C	F	O	0	0
			6	2	3	1		
3	C	1	Total	C	F	O	0	0
			6	2	3	1		
3	C	1	Total	C	F	O	0	0
			6	2	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	F	O	0	0
			6	2	3	1		
3	D	1	Total	C	F	O	0	0
			6	2	3	1		
3	D	1	Total	C	F	O	0	0
			6	2	3	1		

- 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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	D	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		

- Molecule 5 is water.

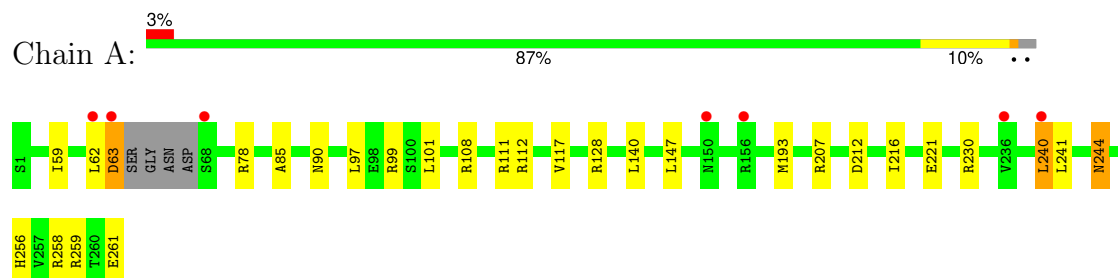
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	190	Total	O	0	0
			190	190		
5	B	217	Total	O	0	0
			217	217		
5	C	219	Total	O	0	0
			219	219		
5	D	222	Total	O	0	0
			222	222		



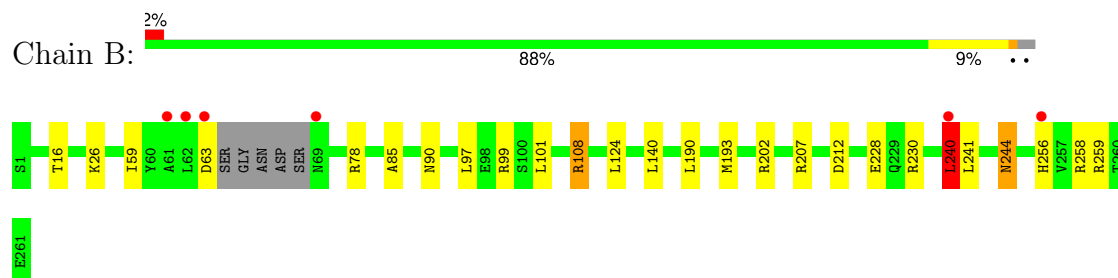
### 3 Residue-property plots [i](#)

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.

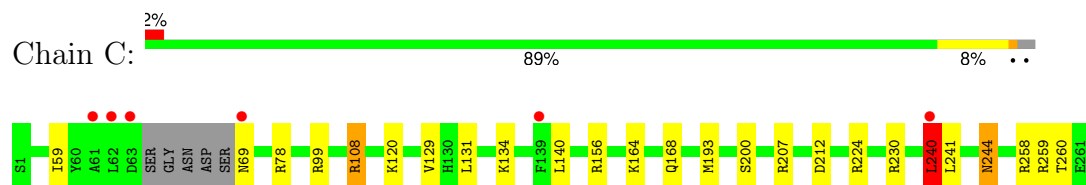
#### • Molecule 1: Ferrous iron transport protein B



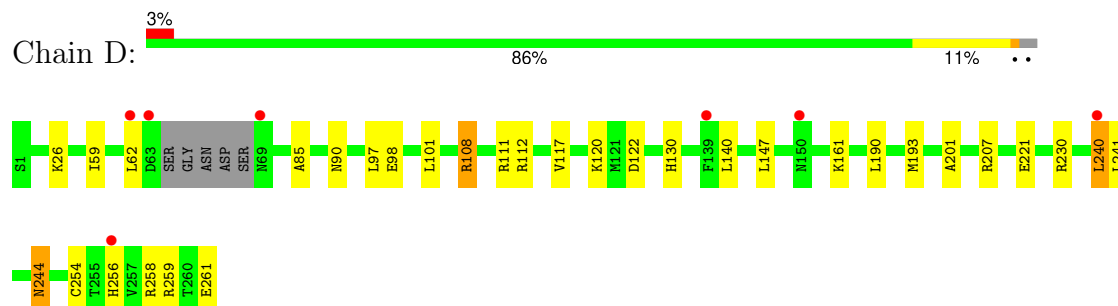
#### • Molecule 1: Ferrous iron transport protein B



#### • Molecule 1: Ferrous iron transport protein B



#### • Molecule 1: Ferrous iron transport protein B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.48Å 101.11Å 301.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.53 – 1.85 43.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.53-1.85) 100.0 (43.53-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.86Å)	Xtriage
Refinement program	REFMAC 4.4.7	Depositor
R, $R_{free}$	0.176 , 0.207 0.186 , 0.218	Depositor DCC
$R_{free}$ test set	6463 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, ETF

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	0.78	2/2062 (0.1%)	0.96	6/2784 (0.2%)
1	B	0.76	1/2056 (0.0%)	0.96	3/2776 (0.1%)
1	C	0.77	2/2056 (0.1%)	0.94	2/2776 (0.1%)
1	D	0.75	0/2056	0.96	4/2776 (0.1%)
All	All	0.77	5/8230 (0.1%)	0.96	15/11112 (0.1%)

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	A	0	5
1	B	0	6
1	C	0	7
1	D	0	4
All	All	0	22

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	MET	SD-CE	-9.19	1.56	1.79
1	A	193	MET	SD-CE	-7.45	1.60	1.79
1	A	240	LEU	CB-CG	5.85	1.65	1.53
1	C	240	LEU	CB-CG	5.47	1.64	1.53
1	B	240	LEU	CB-CG	5.31	1.64	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	ASN	CA-CB-CG	8.92	121.52	112.60
1	D	244	ASN	CA-CB-CG	7.72	120.32	112.60
1	A	244	ASN	CA-CB-CG	7.48	120.08	112.60
1	C	244	ASN	CA-CB-CG	7.00	119.60	112.60
1	A	63	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	90	ASN	CA-CB-CG	5.70	118.30	112.60
1	D	85	ALA	N-CA-C	5.69	118.73	110.42
1	D	90	ASN	CA-CB-CG	5.53	118.13	112.60
1	A	85	ALA	N-CA-C	5.45	117.98	110.35
1	B	90	ASN	CA-CB-CG	5.30	117.90	112.60
1	B	85	ALA	N-CA-C	5.28	117.75	110.35
1	C	69	ASN	CA-CB-CG	5.23	117.83	112.60
1	D	112	ARG	CB-CA-C	-5.06	101.52	109.11
1	A	216	ILE	N-CA-C	5.04	116.49	111.00
1	A	112	ARG	CB-CA-C	-5.01	101.59	109.11

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ARG	Sidechain
1	A	258	ARG	Sidechain
1	A	259	ARG	Sidechain
1	A	78	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	108	ARG	Sidechain
1	B	207	ARG	Sidechain
1	B	258	ARG	Sidechain
1	B	259	ARG	Sidechain
1	B	78	ARG	Sidechain
1	B	99	ARG	Sidechain
1	C	108	ARG	Sidechain
1	C	156	ARG	Sidechain
1	C	207	ARG	Sidechain
1	C	258	ARG	Sidechain
1	C	259	ARG	Sidechain
1	C	78	ARG	Sidechain
1	C	99	ARG	Sidechain
1	D	108	ARG	Sidechain
1	D	207	ARG	Sidechain
1	D	258	ARG	Sidechain
1	D	259	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2034	0	2074	14	0
1	B	2028	0	2069	16	0
1	C	2028	0	2069	13	0
1	D	2028	0	2069	23	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	12	0	16	3	0
3	A	24	0	12	3	0
3	B	36	0	18	6	0
3	C	24	0	12	6	0
3	D	18	0	9	6	0
4	A	20	0	0	0	0
4	B	10	0	0	0	0
4	C	15	0	0	0	0
4	D	25	0	0	1	0
5	A	190	0	0	3	0
5	B	217	0	0	7	1
5	C	219	0	0	1	1
5	D	222	0	0	7	0
All	All	9174	0	8380	72	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 4.

All (72) 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:200:SER:HB2	3:C:302:ETF:H21	1.53	0.89
1:D:256:HIS:HD2	5:D:413:HOH:O	1.64	0.79
1:B:16:THR:HB	3:B:303:ETF:H21	1.66	0.78
3:C:302:ETF:H22	5:C:447:HOH:O	1.84	0.77
1:D:120:LYS:HA	2:D:301:GOL:H2	1.69	0.74
3:D:304:ETF:O	5:D:401:HOH:O	2.06	0.73
1:D:201:ALA:H	3:D:304:ETF:H21	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLU:OE2	5:B:401:HOH:O	2.07	0.71
1:D:244:ASN:HA	5:D:402:HOH:O	1.92	0.68
1:D:221:GLU:H	3:D:305:ETF:H22	1.57	0.68
1:B:244:ASN:HA	5:B:402:HOH:O	1.99	0.62
3:A:306:ETF:O	5:A:401:HOH:O	2.14	0.62
1:A:240:LEU:HB2	5:A:565:HOH:O	2.00	0.61
1:B:16:THR:H	3:B:303:ETF:H21	1.64	0.61
1:A:221:GLU:H	2:A:301:GOL:H2	1.65	0.61
1:A:256:HIS:ND1	5:A:403:HOH:O	2.32	0.58
1:B:16:THR:CB	3:B:303:ETF:H21	2.33	0.58
1:C:224:ARG:HE	3:C:305:ETF:C2	2.18	0.57
1:D:120:LYS:HA	1:D:120:LYS:HE2	1.86	0.57
1:D:117:VAL:HG13	1:D:147:LEU:HB3	1.88	0.55
1:D:122:ASP:HB2	2:D:301:GOL:H12	1.89	0.55
1:B:240:LEU:C	1:B:240:LEU:HD23	2.32	0.55
3:D:304:ETF:H22	5:D:585:HOH:O	2.08	0.54
1:D:240:LEU:C	1:D:240:LEU:HD23	2.33	0.54
5:B:402:HOH:O	1:C:244:ASN:HA	2.09	0.53
1:C:240:LEU:HD23	1:C:240:LEU:C	2.33	0.53
1:D:130:HIS:HE1	1:D:261:GLU:OE1	1.93	0.51
1:B:190:LEU:O	1:B:193:MET:HG2	2.11	0.51
1:D:190:LEU:O	1:D:193:MET:HG2	2.11	0.51
1:A:117:VAL:HG13	1:A:147:LEU:HB3	1.93	0.51
1:D:244:ASN:OD1	5:D:402:HOH:O	2.18	0.51
1:C:129:VAL:HG22	1:C:260:THR:HG22	1.94	0.50
1:A:117:VAL:HG11	1:A:147:LEU:HD23	1.93	0.50
1:D:111:ARG:HH22	2:D:302:GOL:H31	1.78	0.49
3:B:303:ETF:H22	5:B:479:HOH:O	2.12	0.49
1:A:128:ARG:HB3	1:A:261:GLU:HG2	1.93	0.49
1:B:256:HIS:HD2	5:B:568:HOH:O	1.97	0.48
1:D:117:VAL:HG11	1:D:147:LEU:HD23	1.95	0.48
1:C:224:ARG:HE	3:C:305:ETF:H22	1.78	0.47
1:A:111:ARG:NH1	3:A:306:ETF:H22	2.30	0.47
3:B:306:ETF:H22	5:B:559:HOH:O	2.15	0.46
1:B:241:LEU:C	1:B:241:LEU:HD23	2.41	0.46
1:B:202:ARG:H	3:B:306:ETF:H21	1.80	0.46
1:A:241:LEU:C	1:A:241:LEU:HD23	2.40	0.46
1:C:120:LYS:HD2	3:C:304:ETF:H22	1.98	0.46
1:D:221:GLU:N	3:D:305:ETF:H22	2.28	0.46
1:D:241:LEU:C	1:D:241:LEU:HD23	2.41	0.46
1:C:224:ARG:HE	3:C:305:ETF:H21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:HD3	1:C:140:LEU:O	2.17	0.44
1:A:244:ASN:HA	5:D:402:HOH:O	2.17	0.43
1:D:108:ARG:HD3	1:D:140:LEU:O	2.18	0.43
1:D:256:HIS:CD2	5:D:413:HOH:O	2.52	0.43
1:B:108:ARG:HD3	1:B:140:LEU:O	2.18	0.43
1:C:241:LEU:HD23	1:C:241:LEU:C	2.42	0.43
1:A:108:ARG:HD3	1:A:140:LEU:O	2.18	0.43
1:C:164:LYS:HE2	1:C:168:GLN:HE22	1.84	0.43
1:D:193:MET:HE2	1:D:193:MET:HB3	1.89	0.42
1:D:161:LYS:NZ	4:D:310:SO4:O4	2.44	0.42
1:D:201:ALA:H	3:D:304:ETF:C2	2.29	0.42
1:B:212:ASP:OD1	1:B:212:ASP:C	2.62	0.42
1:B:97:LEU:HD22	1:B:101:LEU:HD11	2.01	0.41
1:A:97:LEU:HD22	1:A:101:LEU:HD11	2.01	0.41
1:A:128:ARG:HB3	1:A:261:GLU:CG	2.51	0.41
1:A:212:ASP:OD1	1:A:212:ASP:C	2.64	0.41
1:D:97:LEU:HD22	1:D:101:LEU:HD11	2.03	0.41
1:B:256:HIS:CD2	5:B:568:HOH:O	2.74	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.88	0.40
1:D:98:GLU:HG3	1:D:254:CYS:SG	2.61	0.40
1:C:164:LYS:HE2	1:C:168:GLN:NE2	2.36	0.40
1:C:212:ASP:OD1	1:C:212:ASP:C	2.64	0.40
1:A:111:ARG:HH11	3:A:306:ETF:C2	2.34	0.40
1:B:193:MET:HE2	1:B:193:MET:HB3	1.91	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)
5:B:589:HOH:O	5:C:539:HOH:O[5_545]	2.01	0.19

## 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	253/261 (97%)	251 (99%)	2 (1%)	0	100	100
1	B	252/261 (97%)	251 (100%)	1 (0%)	0	100	100
1	C	252/261 (97%)	249 (99%)	3 (1%)	0	100	100
1	D	252/261 (97%)	250 (99%)	2 (1%)	0	100	100
All	All	1009/1044 (97%)	1001 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	222/225 (99%)	218 (98%)	4 (2%)	51	40
1	B	221/225 (98%)	216 (98%)	5 (2%)	44	30
1	C	221/225 (98%)	216 (98%)	5 (2%)	44	30
1	D	221/225 (98%)	216 (98%)	5 (2%)	44	30
All	All	885/900 (98%)	866 (98%)	19 (2%)	47	33

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	62	LEU
1	A	63	ASP
1	A	230	ARG
1	B	26	LYS
1	B	59	ILE
1	B	63	ASP
1	B	230	ARG
1	B	240	LEU
1	C	59	ILE
1	C	131	LEU

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Mol	Chain	Res	Type
1	C	134	LYS
1	C	230	ARG
1	C	240	LEU
1	D	26	LYS
1	D	59	ILE
1	D	62	LEU
1	D	230	ARG
1	D	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	90	ASN
1	A	106	GLN
1	A	130	HIS
1	A	256	HIS
1	B	31	ASN
1	B	106	GLN
1	B	130	HIS
1	C	130	HIS
1	C	168	GLN
1	C	251	HIS
1	D	31	ASN
1	D	106	GLN
1	D	130	HIS
1	D	244	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

37 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	$\# Z  > 2$
3	ETF	B	302	-	5,5,5	0.39	0	7,7,7	0.35	0
2	GOL	D	301	-	5,5,5	0.11	0	5,5,5	0.36	0
4	SO4	D	310	-	4,4,4	0.35	0	6,6,6	0.06	0
3	ETF	C	305	-	5,5,5	0.28	0	7,7,7	0.27	0
3	ETF	D	303	-	5,5,5	0.31	0	7,7,7	0.32	0
3	ETF	B	305	-	5,5,5	0.25	0	7,7,7	0.24	0
3	ETF	A	305	-	5,5,5	0.26	0	7,7,7	0.11	0
4	SO4	C	306	-	4,4,4	0.37	0	6,6,6	0.16	0
2	GOL	D	302	-	5,5,5	0.10	0	5,5,5	0.34	0
4	SO4	D	309	-	4,4,4	0.36	0	6,6,6	0.18	0
3	ETF	B	304	-	5,5,5	0.26	0	7,7,7	0.17	0
3	ETF	A	306	-	5,5,5	0.49	0	7,7,7	0.41	0
2	GOL	A	301	-	5,5,5	0.12	0	5,5,5	0.32	0
4	SO4	C	307	-	4,4,4	0.29	0	6,6,6	0.14	0
2	GOL	C	301	-	5,5,5	0.12	0	5,5,5	0.41	0
4	SO4	D	306	-	4,4,4	0.39	0	6,6,6	0.15	0
4	SO4	B	308	-	4,4,4	0.27	0	6,6,6	0.13	0
3	ETF	C	303	-	5,5,5	0.28	0	7,7,7	0.16	0
3	ETF	D	304	-	5,5,5	0.47	0	7,7,7	0.22	0
3	ETF	C	302	-	5,5,5	0.34	0	7,7,7	0.34	0
2	GOL	A	302	-	5,5,5	0.10	0	5,5,5	0.31	0
4	SO4	D	307	-	4,4,4	0.29	0	6,6,6	0.12	0
3	ETF	A	303	-	5,5,5	0.27	0	7,7,7	0.35	0
3	ETF	B	307	-	5,5,5	0.28	0	7,7,7	0.14	0
3	ETF	C	304	-	5,5,5	0.45	0	7,7,7	0.57	0
4	SO4	A	308	-	4,4,4	0.30	0	6,6,6	0.10	0
4	SO4	A	310	-	4,4,4	0.37	0	6,6,6	0.16	0
4	SO4	C	308	-	4,4,4	0.34	0	6,6,6	0.25	0
3	ETF	A	304	-	5,5,5	0.32	0	7,7,7	0.15	0
3	ETF	B	306	-	5,5,5	0.33	0	7,7,7	0.31	0
4	SO4	A	307	-	4,4,4	0.33	0	6,6,6	0.13	0
2	GOL	B	301	-	5,5,5	0.13	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	B	309	-	4,4,4	0.31	0	6,6,6	0.12	0
4	SO4	D	308	-	4,4,4	0.35	0	6,6,6	0.12	0
3	ETF	D	305	-	5,5,5	0.23	0	7,7,7	0.29	0
3	ETF	B	303	-	5,5,5	0.25	0	7,7,7	0.35	0
4	SO4	A	309	-	4,4,4	0.28	0	6,6,6	0.09	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
3	ETF	B	302	-	-	3/3/3/3	-
2	GOL	D	301	-	-	3/4/4/4	-
3	ETF	C	305	-	-	3/3/3/3	-
3	ETF	D	303	-	-	3/3/3/3	-
3	ETF	B	305	-	-	3/3/3/3	-
3	ETF	A	305	-	-	3/3/3/3	-
2	GOL	D	302	-	-	0/4/4/4	-
3	ETF	B	304	-	-	3/3/3/3	-
3	ETF	A	306	-	-	0/3/3/3	-
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-
3	ETF	C	303	-	-	3/3/3/3	-
3	ETF	D	304	-	-	3/3/3/3	-
3	ETF	C	302	-	-	0/3/3/3	-
2	GOL	A	302	-	-	2/4/4/4	-
3	ETF	A	303	-	-	3/3/3/3	-
3	ETF	B	307	-	-	3/3/3/3	-
3	ETF	C	304	-	-	0/3/3/3	-
3	ETF	A	304	-	-	3/3/3/3	-
3	ETF	B	306	-	-	3/3/3/3	-
2	GOL	B	301	-	-	3/4/4/4	-
3	ETF	D	305	-	-	0/3/3/3	-
3	ETF	B	303	-	-	3/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	O1-C1-C2-C3
2	C	301	GOL	C1-C2-C3-O3
2	A	302	GOL	O2-C2-C3-O3
2	D	301	GOL	O2-C2-C3-O3
3	A	305	ETF	F2-C1-C2-O
3	A	305	ETF	F3-C1-C2-O
3	B	304	ETF	F1-C1-C2-O
3	B	305	ETF	F1-C1-C2-O
3	B	305	ETF	F2-C1-C2-O
3	B	307	ETF	F1-C1-C2-O
3	B	307	ETF	F2-C1-C2-O
3	C	303	ETF	F3-C1-C2-O
3	D	304	ETF	F1-C1-C2-O
3	D	304	ETF	F2-C1-C2-O
3	A	303	ETF	F2-C1-C2-O
3	A	304	ETF	F2-C1-C2-O
3	B	302	ETF	F2-C1-C2-O
3	B	302	ETF	F3-C1-C2-O
3	B	306	ETF	F1-C1-C2-O
3	C	303	ETF	F1-C1-C2-O
3	C	303	ETF	F2-C1-C2-O
3	C	305	ETF	F2-C1-C2-O
3	D	303	ETF	F1-C1-C2-O
3	D	303	ETF	F2-C1-C2-O
2	A	302	GOL	C1-C2-C3-O3
2	D	301	GOL	C1-C2-C3-O3
3	A	305	ETF	F1-C1-C2-O
3	B	302	ETF	F1-C1-C2-O
3	B	304	ETF	F3-C1-C2-O
3	B	305	ETF	F3-C1-C2-O
3	B	307	ETF	F3-C1-C2-O
3	D	303	ETF	F3-C1-C2-O
3	D	304	ETF	F3-C1-C2-O
3	A	304	ETF	F1-C1-C2-O
3	B	303	ETF	F1-C1-C2-O
3	B	304	ETF	F2-C1-C2-O
3	C	305	ETF	F3-C1-C2-O
3	A	303	ETF	F1-C1-C2-O
3	A	304	ETF	F3-C1-C2-O
3	B	306	ETF	F2-C1-C2-O

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Mol	Chain	Res	Type	Atoms
3	C	305	ETF	F1-C1-C2-O
2	B	301	GOL	O1-C1-C2-O2
2	C	301	GOL	O2-C2-C3-O3
3	A	303	ETF	F3-C1-C2-O
3	B	306	ETF	F3-C1-C2-O
3	B	303	ETF	F3-C1-C2-O
3	B	303	ETF	F2-C1-C2-O
2	B	301	GOL	O2-C2-C3-O3
2	D	301	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	GOL	2	0
4	D	310	SO4	1	0
3	C	305	ETF	3	0
2	D	302	GOL	1	0
3	A	306	ETF	3	0
2	A	301	GOL	1	0
3	D	304	ETF	4	0
3	C	302	ETF	2	0
3	C	304	ETF	1	0
3	B	306	ETF	2	0
3	D	305	ETF	2	0
3	B	303	ETF	4	0

## 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	257/261 (98%)	-0.01	7 (2%) 56 59	21, 34, 66, 121	0
1	B	256/261 (98%)	-0.10	6 (2%) 61 64	21, 33, 60, 97	0
1	C	256/261 (98%)	-0.08	6 (2%) 61 64	20, 34, 62, 91	0
1	D	256/261 (98%)	-0.03	7 (2%) 56 59	21, 32, 62, 104	0
All	All	1025/1044 (98%)	-0.05	26 (2%) 58 62	20, 33, 62, 121	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	62	LEU	4.0
1	C	63	ASP	3.7
1	A	63	ASP	3.7
1	C	69	ASN	3.6
1	A	68	SER	3.4
1	B	63	ASP	3.1
1	D	63	ASP	3.1
1	B	240	LEU	2.9
1	A	240	LEU	2.8
1	D	240	LEU	2.8
1	C	61	ALA	2.7
1	C	62	LEU	2.5
1	B	69	ASN	2.4
1	B	62	LEU	2.3
1	D	69	ASN	2.3
1	A	62	LEU	2.3
1	C	240	LEU	2.3
1	B	256	HIS	2.2
1	D	139	PHE	2.2
1	C	139	PHE	2.2
1	A	236	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	2.1
1	D	256	HIS	2.1
1	D	150	ASN	2.1
1	A	150	ASN	2.1
1	A	156	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	GOL	A	302	6/6	0.73	0.17	53,87,95,104	0
2	GOL	D	302	6/6	0.75	0.15	63,68,72,85	0
3	ETF	A	304	6/6	0.76	0.12	64,74,90,113	0
3	ETF	B	302	6/6	0.76	0.20	44,78,98,107	0
3	ETF	B	307	6/6	0.76	0.13	57,76,91,126	0
3	ETF	C	304	6/6	0.76	0.20	43,83,119,135	0
3	ETF	A	303	6/6	0.80	0.15	54,67,82,86	0
3	ETF	D	303	6/6	0.80	0.16	53,69,93,125	0
4	SO4	A	309	5/5	0.81	0.09	64,69,99,143	0
3	ETF	C	305	6/6	0.82	0.11	54,67,71,71	0
2	GOL	D	301	6/6	0.83	0.16	60,66,88,89	0
2	GOL	B	301	6/6	0.86	0.13	49,55,72,75	0
4	SO4	D	310	5/5	0.86	0.09	75,81,110,183	0
2	GOL	C	301	6/6	0.87	0.14	48,54,74,78	0
4	SO4	A	310	5/5	0.87	0.21	31,52,84,124	5
3	ETF	D	305	6/6	0.87	0.11	48,55,94,109	0
3	ETF	B	305	6/6	0.88	0.15	53,75,101,118	0
3	ETF	B	306	6/6	0.88	0.12	33,49,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	307	5/5	0.89	0.11	48,61,71,117	0
2	GOL	A	301	6/6	0.89	0.11	51,52,54,80	0
3	ETF	C	303	6/6	0.90	0.14	59,62,83,90	0
3	ETF	B	304	6/6	0.91	0.15	58,59,80,95	0
4	SO4	D	309	5/5	0.91	0.10	34,48,58,82	5
4	SO4	B	308	5/5	0.91	0.09	41,55,60,82	0
4	SO4	C	307	5/5	0.92	0.10	41,51,72,147	0
3	ETF	A	306	6/6	0.92	0.12	40,43,77,80	0
3	ETF	A	305	6/6	0.93	0.16	53,68,89,90	0
4	SO4	D	308	5/5	0.93	0.11	66,68,86,94	0
4	SO4	A	308	5/5	0.93	0.10	46,58,85,88	0
3	ETF	C	302	6/6	0.93	0.09	31,41,58,59	0
4	SO4	B	309	5/5	0.94	0.07	54,66,66,83	0
4	SO4	A	307	5/5	0.94	0.08	39,40,53,59	0
4	SO4	D	306	5/5	0.96	0.07	35,39,50,56	0
3	ETF	B	303	6/6	0.96	0.08	15,31,43,52	0
4	SO4	C	306	5/5	0.96	0.06	35,43,46,56	0
3	ETF	D	304	6/6	0.96	0.08	24,42,55,75	0
4	SO4	C	308	5/5	0.96	0.07	43,47,51,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.