



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:46 PM GMT

PDB ID : 4MOJ  
Title : Pyranose 2-oxidase H450G/V546C double mutant with 2-fluorinated glucose  
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.  
Deposited on : 2013-09-12  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

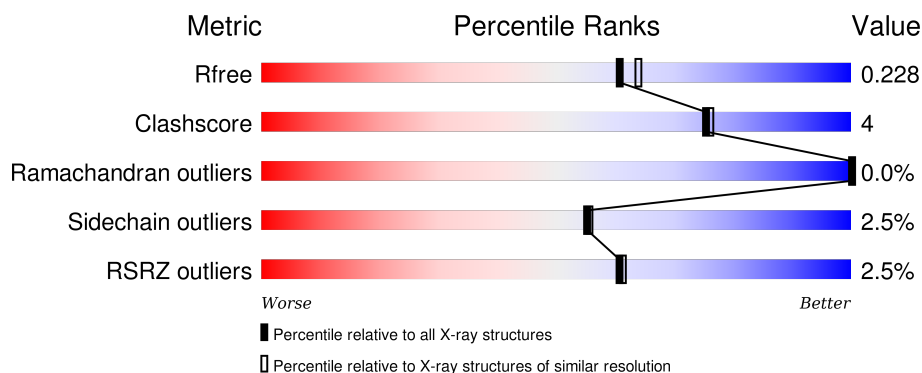
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	633	 3% 83% 7% • 9%
1	B	633	 2% 81% 9% • 9%
1	C	633	 3% 79% 11% 9%
1	D	633	 2% 84% 7% • 9%

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
4	1PE	B	704	-	-	-	X
4	1PE	C	803	-	-	-	X
5	MES	A	804	-	-	-	X
5	MES	B	701	-	-	-	X
5	MES	D	804	-	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20415 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 Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4535	2862	775	872	26			
1	B	576	Total	C	N	O	S	0	1	0
			4541	2866	776	873	26			
1	C	574	Total	C	N	O	S	0	0	0
			4519	2853	773	868	25			
1	D	575	Total	C	N	O	S	0	0	0
			4526	2857	774	870	25			

There are 56 discrepancies between the modelled and reference sequences:

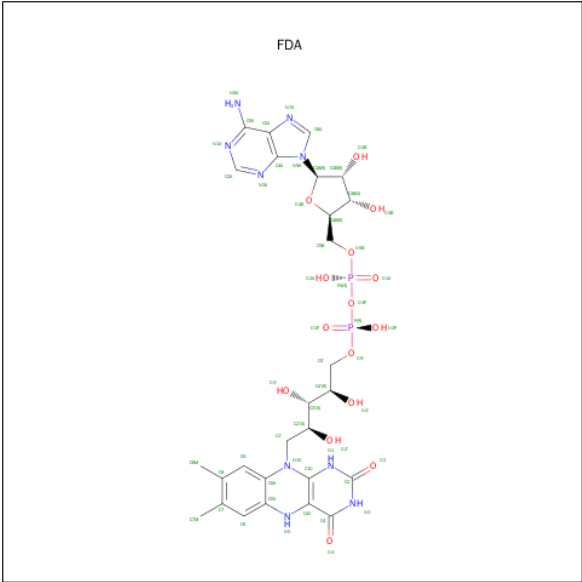
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
A	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
A	546	CYS	VAL	ENGINEERED MUTATION	UNP Q7ZA32
A	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
A	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
A	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
B	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
B	546	CYS	VAL	ENGINEERED MUTATION	UNP Q7ZA32
B	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32

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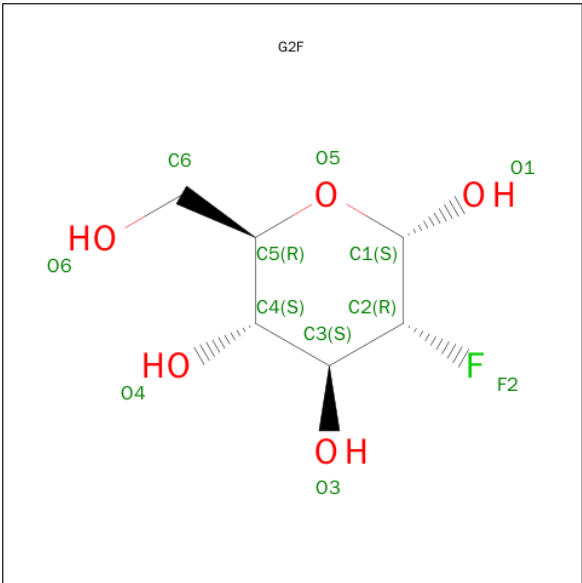
Chain	Residue	Modelled	Actual	Comment	Reference
B	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
B	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
C	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
C	546	CYS	VAL	ENGINEERED MUTATION	UNP Q7ZA32
C	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
C	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
C	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
D	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
D	546	CYS	VAL	ENGINEERED MUTATION	UNP Q7ZA32
D	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
D	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
D	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



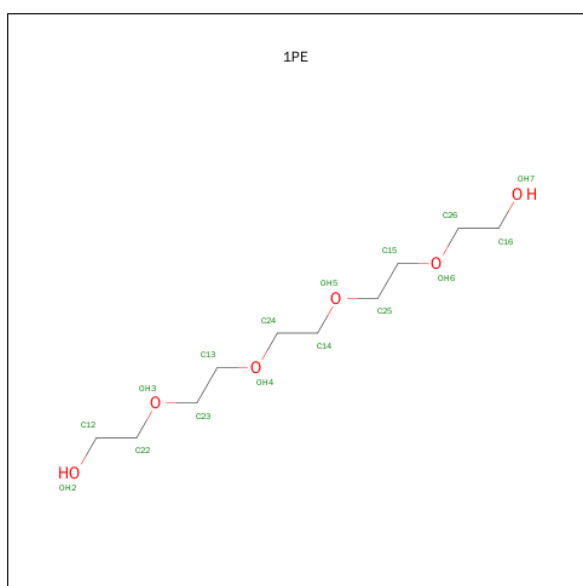
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SUGAR (2-DEOXY-2-FLUORO-ALPHA-D-GLUCOPYRANOSE) (three-letter code: G2F) (formula: C<sub>6</sub>H<sub>11</sub>FO<sub>5</sub>).



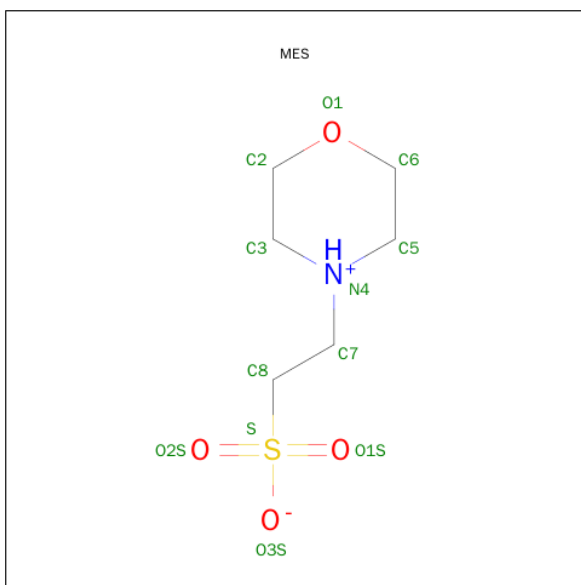
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 6	F 1	O 5	0	0
3	B	1	Total 12	C 6	F 1	O 5	0	0
3	C	1	Total 12	C 6	F 1	O 5	0	0
3	D	1	Total 12	C 6	F 1	O 5	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $\text{C}_{10}\text{H}_{22}\text{O}_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 12	C 8	O 4	0	0
4	B	1	Total 16	C 10	O 6	0	0
4	C	1	Total 16	C 10	O 6	0	0
4	D	1	Total 16	C 10	O 6	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is water.

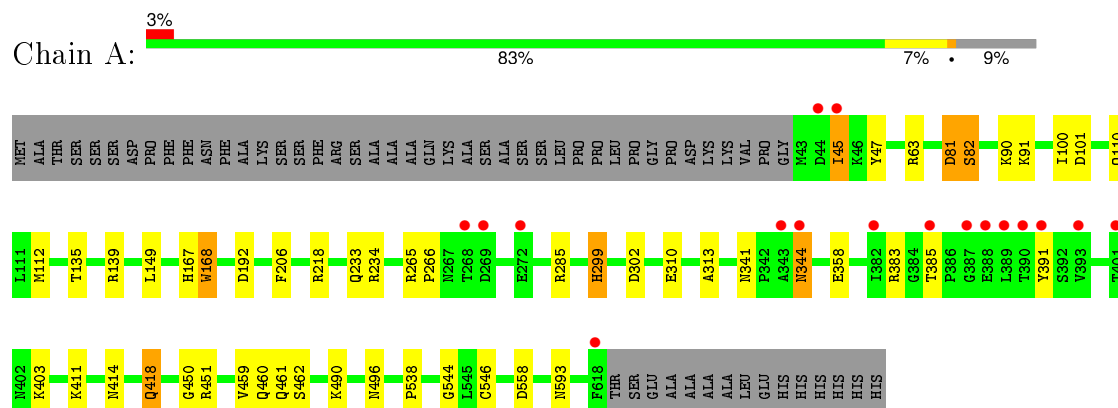
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	466	Total	O	0	0
			466	466		
6	B	561	Total	O	0	0
			561	561		
6	C	378	Total	O	0	0
			378	378		
6	D	521	Total	O	0	0
			521	521		



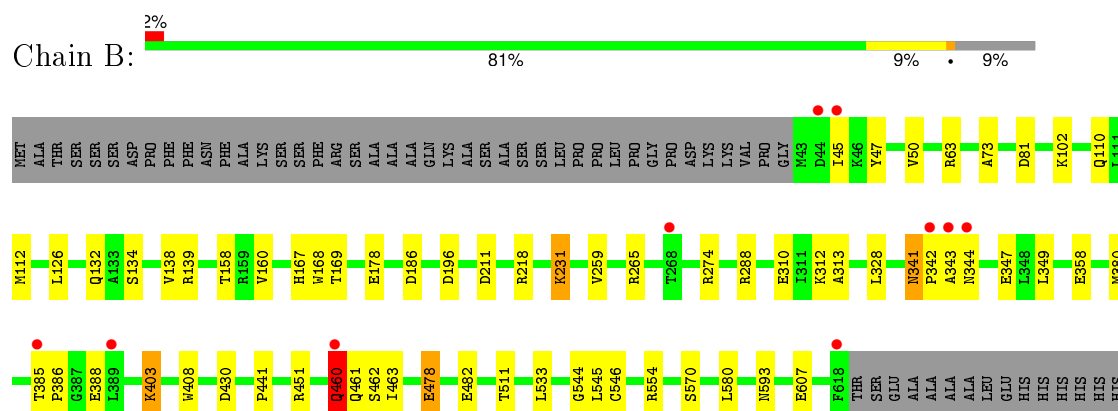
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

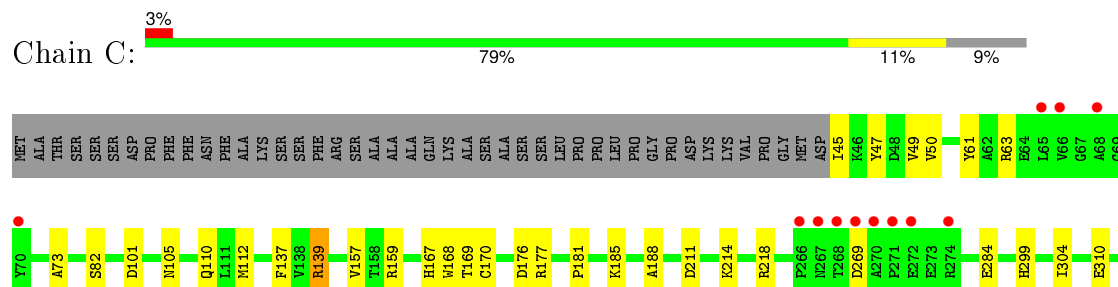
#### • Molecule 1: Pyranose 2-oxidase

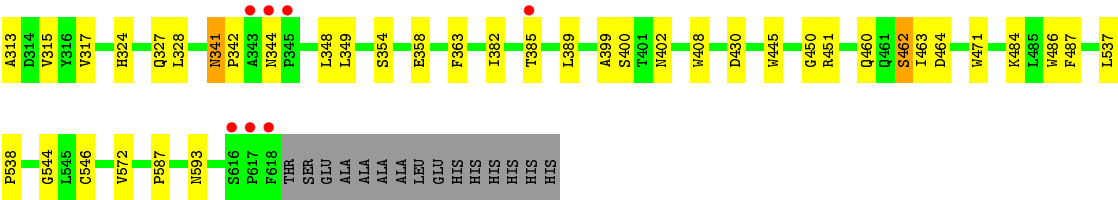


#### • Molecule 1: Pyranose 2-oxidase

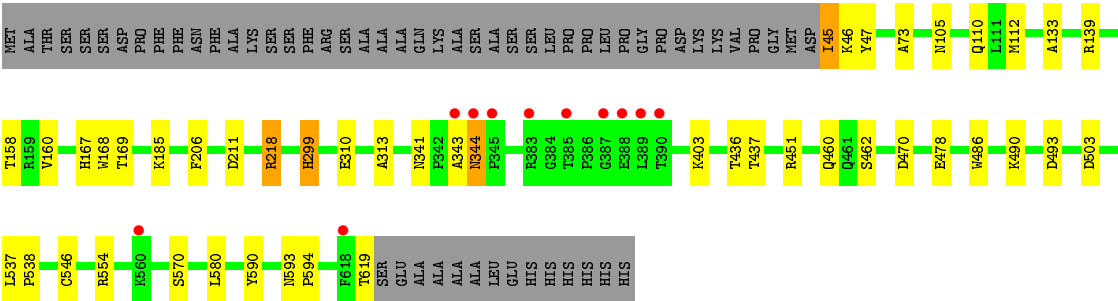
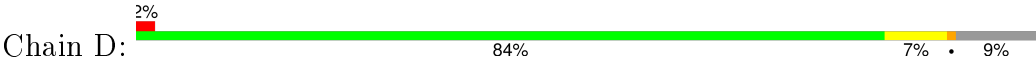


#### • Molecule 1: Pyranose 2-oxidase





● Molecule 1: Pyranose 2-oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.08Å 102.52Å 137.34Å 90.00° 90.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 49.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.00) 99.8 (49.85-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.172 , 0.222 0.180 , 0.228	Depositor DCC
$R_{free}$ test set	3747 reflections (2.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.0	EDS
Estimated twinning fraction	0.014 for -k,-h,-l 0.015 for k,h,-l 0.024 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 186782 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FDA, G2F, MES, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.02	4/4650 (0.1%)	0.98	10/6321 (0.2%)
1	B	1.04	4/4659 (0.1%)	1.01	17/6333 (0.3%)
1	C	0.89	3/4634 (0.1%)	0.89	4/6300 (0.1%)
1	D	0.96	3/4641 (0.1%)	0.95	10/6310 (0.2%)
All	All	0.98	14/18584 (0.1%)	0.96	41/25264 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	GLU	CD-OE2	8.54	1.35	1.25
1	A	82	SER	CB-OG	8.28	1.53	1.42
1	B	546	CYS	CB-SG	-8.23	1.68	1.82
1	D	546	CYS	CB-SG	-6.91	1.70	1.82
1	B	482	GLU	CD-OE1	6.79	1.33	1.25
1	B	134	SER	CB-OG	-6.59	1.33	1.42
1	C	546	CYS	CB-SG	-6.26	1.71	1.82
1	A	546	CYS	CB-SG	-6.06	1.72	1.82
1	B	478	GLU	CD-OE1	5.41	1.31	1.25
1	A	82	SER	N-CA	5.28	1.56	1.46
1	D	486	TRP	CD2-CE2	5.23	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	TRP	CD2-CE2	5.16	1.47	1.41
1	C	486	TRP	CD2-CE2	5.14	1.47	1.41
1	C	445	TRP	CG-CD2	5.11	1.52	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH2	-13.02	113.79	120.30
1	D	139	ARG	NE-CZ-NH2	-11.83	114.39	120.30
1	B	81	ASP	CB-CG-OD1	-8.61	110.55	118.30
1	D	139	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	B	211	ASP	CB-CG-OD1	8.43	125.89	118.30
1	A	139	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	211	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	D	211	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	139	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	81	ASP	CB-CG-OD2	7.35	124.92	118.30
1	B	196	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	546	CYS	CA-CB-SG	-6.85	101.67	114.00
1	A	82	SER	CA-CB-OG	6.55	128.89	111.20
1	D	218	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	139	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	503	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	464	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	B	451	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	192	ASP	CB-CG-OD1	6.05	123.74	118.30
1	C	101	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	554	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	B	349	LEU	CA-CB-CG	5.90	128.88	115.30
1	B	288	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	503	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	63	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	139	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	D	470	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	D	554	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	380	MET	CG-SD-CE	-5.60	91.24	100.20
1	A	234	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	546	CYS	CA-CB-SG	-5.58	103.96	114.00
1	B	265	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	302	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	81	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	558	ASP	CB-CG-OD2	5.36	123.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	B	274	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	102	LYS	CD-CE-NZ	-5.18	99.78	111.70
1	C	63	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	554	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	231	LYS	CD-CE-NZ	5.01	123.21	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASP	Peptide
1	B	138	VAL	Peptide
1	D	436	THR	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4535	0	4380	31	0
1	B	4541	0	4388	36	0
1	C	4519	0	4367	45	0
1	D	4526	0	4374	24	0
2	A	53	0	30	0	0
2	B	53	0	30	2	0
2	C	53	0	29	2	0
2	D	53	0	30	2	0
3	A	12	0	11	0	0
3	B	12	0	11	1	0
3	C	12	0	11	1	0
3	D	12	0	11	1	0
4	A	12	0	14	0	0
4	B	16	0	22	0	0
4	C	16	0	22	0	0
4	D	16	0	22	4	0
5	A	12	0	13	0	0
5	B	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	24	0	26	10	0
6	A	466	0	0	8	0
6	B	561	0	0	6	0
6	C	378	0	0	6	0
6	D	521	0	0	4	0
All	All	20415	0	17804	140	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 4.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:HIS:CE1	1:D:310:GLU:HG2	1.91	1.06
1:A:45:ILE:HD12	1:A:45:ILE:H	1.15	1.05
1:B:460[B]:GLN:HE22	1:B:463:ILE:H	0.93	0.89
1:B:460[B]:GLN:NE2	1:B:463:ILE:H	1.68	0.89
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.20	0.89
1:B:385:THR:HG23	1:B:388:GLU:OE1	1.76	0.85
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.26	0.84
1:A:414:ASN:O	1:A:418:GLN:HG2	1.80	0.82
1:D:343:ALA:C	1:D:344:ASN:HD22	1.84	0.81
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.29	0.79
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.30	0.77
1:A:45:ILE:CD1	1:A:45:ILE:H	1.92	0.76
1:B:460[B]:GLN:HE22	1:B:463:ILE:N	1.77	0.76
1:B:45:ILE:HG22	6:B:1277:HOH:O	1.85	0.75
1:A:101:ASP:HB2	6:A:1321:HOH:O	1.88	0.74
1:D:133:ALA:HB2	5:D:804:MES:O3S	1.89	0.73
1:A:460:GLN:NE2	6:A:1217:HOH:O	2.23	0.71
1:B:385:THR:CG2	1:B:388:GLU:OE1	2.37	0.71
1:A:45:ILE:N	1:A:45:ILE:HD12	1.99	0.69
1:D:45:ILE:HG22	1:D:46:LYS:H	1.57	0.69
1:C:450:GLY:O	1:C:451:ARG:HD2	1.93	0.69
5:D:804:MES:H32	5:D:804:MES:O1S	1.93	0.69
1:B:341:ASN:HD22	1:B:341:ASN:C	1.95	0.69
1:C:463:ILE:HD13	5:D:804:MES:H81	1.76	0.67
1:A:462:SER:OG	5:B:701:MES:H61	1.95	0.67
1:B:341:ASN:ND2	6:B:1276:HOH:O	2.29	0.64
1:D:344:ASN:N	1:D:344:ASN:HD22	1.96	0.63
1:C:349:LEU:HD21	1:C:572:VAL:HG13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HA	6:B:1277:HOH:O	2.01	0.60
1:B:607:GLU:HG3	6:B:1246:HOH:O	2.01	0.60
1:A:101:ASP:OD2	1:A:459:VAL:HG21	2.01	0.60
1:C:176:ASP:HB2	6:C:1161:HOH:O	2.01	0.59
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.68	0.59
1:B:63:ARG:HD2	1:B:259:VAL:O	2.04	0.58
1:B:341:ASN:ND2	1:B:341:ASN:C	2.57	0.58
1:C:177:ARG:NH2	1:C:188:ALA:HB1	2.19	0.58
1:C:47:TYR:O	1:C:313:ALA:HA	2.04	0.57
1:A:90:LYS:NZ	1:A:110:GLN:OE1	2.33	0.57
1:C:82:SER:N	6:C:963:HOH:O	2.38	0.56
1:D:47:TYR:CE2	1:D:73:ALA:HB2	2.40	0.56
1:A:135:THR:HG22	4:D:803:1PE:C22	2.36	0.56
1:A:285:ARG:HD2	6:A:1282:HOH:O	2.06	0.56
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.89	0.55
1:A:135:THR:HG22	4:D:803:1PE:H222	1.90	0.54
1:B:126:LEU:HD12	1:B:132:GLN:HG3	1.90	0.53
1:A:299:HIS:CE1	1:A:310:GLU:HG3	2.43	0.53
1:B:126:LEU:HD12	1:B:132:GLN:CG	2.38	0.53
1:D:133:ALA:H	5:D:804:MES:H72	1.73	0.53
1:B:310:GLU:OE1	1:B:312:LYS:NZ	2.41	0.53
1:A:218:ARG:HD2	6:A:1001:HOH:O	2.07	0.53
1:D:133:ALA:HA	6:D:1407:HOH:O	2.08	0.53
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.90	0.52
1:D:537:LEU:HB3	1:D:538:PRO:HD2	1.92	0.52
1:C:157:VAL:HG22	6:C:1176:HOH:O	2.11	0.51
2:B:702:FDA:N5	3:B:703:G2F:H3	2.25	0.51
1:C:299:HIS:CD2	1:C:310:GLU:HB3	2.46	0.50
1:A:459:VAL:HG13	1:A:461:GLN:HE21	1.76	0.50
1:C:211:ASP:O	1:C:214:LYS:HG2	2.11	0.49
1:C:49:VAL:HG22	1:C:315:VAL:HB	1.95	0.49
1:B:460[B]:GLN:HG3	1:B:533:LEU:HD21	1.95	0.49
1:C:463:ILE:CD1	5:D:804:MES:H81	2.43	0.49
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.12	0.49
1:A:91:LYS:HD2	1:A:100:ILE:HD11	1.93	0.49
1:C:105:ASN:HB3	1:D:105:ASN:O	2.13	0.48
1:B:460[B]:GLN:HB2	6:B:1204:HOH:O	2.14	0.48
1:A:149:LEU:HD22	5:D:804:MES:H62	1.94	0.48
1:A:233:GLN:NE2	6:A:1252:HOH:O	2.27	0.48
1:C:358:GLU:HG2	1:C:544:GLY:HA2	1.96	0.48
1:B:342:PRO:HD2	6:B:1276:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG21	1:C:324:HIS:CE1	2.48	0.47
1:D:47:TYR:CD2	1:D:73:ALA:HB2	2.49	0.47
1:A:450:GLY:O	1:A:451:ARG:HD2	2.14	0.47
1:B:341:ASN:HD21	1:B:343:ALA:HB3	1.80	0.47
1:C:382:ILE:HD13	6:C:1038:HOH:O	2.15	0.46
1:B:460[A]:GLN:HG3	1:B:461:GLN:N	2.31	0.46
1:D:570:SER:HB3	1:D:580:LEU:O	2.16	0.46
1:C:159:ARG:HA	2:C:801:FDA:O2B	2.16	0.46
1:B:570:SER:HB3	1:B:580:LEU:O	2.16	0.46
1:B:169:THR:HB	2:B:702:FDA:O4	2.16	0.46
1:C:284:GLU:C	1:C:328:LEU:CD1	2.85	0.46
2:D:801:FDA:N5	3:D:802:G2F:H3	2.30	0.46
1:A:344:ASN:CG	1:A:344:ASN:O	2.54	0.46
1:B:545:LEU:HA	1:B:545:LEU:HD12	1.72	0.46
1:C:341:ASN:HD22	1:C:341:ASN:C	2.19	0.45
1:B:385:THR:HA	1:B:386:PRO:HD3	1.85	0.45
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.99	0.45
1:C:389:LEU:HA	1:C:389:LEU:HD12	1.72	0.45
1:C:284:GLU:O	1:C:328:LEU:CD1	2.65	0.44
1:C:137:PHE:CE2	1:C:139:ARG:HG3	2.52	0.44
1:C:463:ILE:CD1	5:D:804:MES:C8	2.95	0.44
1:D:169:THR:HB	2:D:801:FDA:O4	2.18	0.43
1:C:47:TYR:CE2	1:C:73:ALA:HB2	2.53	0.43
1:A:47:TYR:O	1:A:313:ALA:HA	2.18	0.43
5:D:805:MES:H51	5:D:805:MES:H82	1.86	0.43
1:C:463:ILE:HD12	5:D:804:MES:H82	2.00	0.43
1:D:47:TYR:O	1:D:313:ALA:HA	2.18	0.43
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.18	0.43
1:D:45:ILE:HG22	1:D:46:LYS:N	2.28	0.43
2:C:801:FDA:N5	3:C:802:G2F:H3	2.33	0.43
1:A:299:HIS:CE1	1:A:310:GLU:CG	3.01	0.43
1:B:403:LYS:HD2	1:B:403:LYS:N	2.33	0.43
1:C:284:GLU:O	1:C:328:LEU:HD12	2.19	0.43
1:C:460:GLN:NE2	1:C:462:SER:HB2	2.34	0.43
1:A:135:THR:HG22	4:D:803:1PE:H221	2.00	0.43
1:C:399:ALA:HB3	1:C:402:ASN:OD1	2.19	0.43
1:B:158:THR:HG22	1:B:160:VAL:HG22	2.01	0.43
1:B:358:GLU:HG2	1:B:544:GLY:HA2	2.01	0.43
1:D:451:ARG:NH2	6:D:1239:HOH:O	2.52	0.43
1:D:344:ASN:N	1:D:344:ASN:ND2	2.66	0.42
1:D:493:ASP:HB2	6:D:1382:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ARG:O	1:A:391:TYR:HA	2.20	0.42
1:A:82:SER:HB2	6:A:1013:HOH:O	2.19	0.42
1:D:437:THR:O	1:D:437:THR:HG23	2.19	0.42
1:D:218:ARG:HD2	6:D:968:HOH:O	2.18	0.42
1:B:328:LEU:HD23	1:B:328:LEU:C	2.40	0.42
1:C:50:VAL:HG12	1:C:73:ALA:HB3	2.02	0.42
1:B:47:TYR:CD2	1:B:73:ALA:HB2	2.55	0.42
1:A:358:GLU:HG2	1:A:544:GLY:HA2	2.02	0.42
1:C:167:HIS:CD2	1:C:167:HIS:C	2.93	0.41
4:D:803:1PE:H222	4:D:803:1PE:H132	1.79	0.41
1:A:411:LYS:HD3	6:A:1275:HOH:O	2.19	0.41
1:C:61:TYR:CG	1:C:317:VAL:HG11	2.55	0.41
1:C:181:PRO:HB3	1:C:587:PRO:HG2	2.01	0.41
1:B:478:GLU:HG3	1:B:511:THR:OG1	2.19	0.41
1:B:126:LEU:CD1	1:B:132:GLN:CG	2.99	0.41
1:D:133:ALA:HB2	5:D:804:MES:S	2.60	0.41
1:D:590:TYR:CE2	1:D:594:PRO:HB3	2.56	0.41
1:C:327:GLN:HB2	1:C:487:PHE:CE1	2.55	0.41
1:C:363:PHE:HA	1:C:471:TRP:O	2.20	0.41
1:C:349:LEU:HD21	1:C:572:VAL:CG1	2.49	0.41
1:C:342:PRO:C	1:C:344:ASN:H	2.24	0.41
1:B:178:GLU:OE1	1:B:441:PRO:HG3	2.21	0.41
1:C:354:SER:OG	1:C:484:LYS:NZ	2.53	0.41
1:A:82:SER:HB3	6:A:1040:HOH:O	2.20	0.41
1:A:265:ARG:HA	1:A:266:PRO:C	2.42	0.41
1:C:348:LEU:HD22	6:C:1269:HOH:O	2.21	0.40
1:B:385:THR:HG21	1:B:388:GLU:OE1	2.21	0.40
1:C:537:LEU:HB3	1:C:538:PRO:HD2	2.04	0.40
1:C:169:THR:O	1:C:170:CYS:HB2	2.22	0.40
1:C:304:ILE:HG12	6:C:1134:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 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	574/633 (91%)	559 (97%)	15 (3%)	0	100	100
1	B	575/633 (91%)	555 (96%)	18 (3%)	2 (0%)	46	41
1	C	572/633 (90%)	554 (97%)	18 (3%)	0	100	100
1	D	573/633 (90%)	553 (96%)	20 (4%)	0	100	100
All	All	2294/2532 (91%)	2221 (97%)	71 (3%)	2 (0%)	100	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	460[A]	GLN
1	B	460[B]	GLN

### 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	503/547 (92%)	490 (97%)	13 (3%)	54	54
1	B	504/547 (92%)	491 (97%)	13 (3%)	54	54
1	C	501/547 (92%)	490 (98%)	11 (2%)	60	62
1	D	502/547 (92%)	488 (97%)	14 (3%)	51	50
All	All	2010/2188 (92%)	1959 (98%)	51 (2%)	55	55

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	112	MET
1	A	168	TRP
1	A	206	PHE
1	A	299	HIS
1	A	341	ASN

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Mol	Chain	Res	Type
1	A	344	ASN
1	A	385	THR
1	A	403	LYS
1	A	418	GLN
1	A	490	LYS
1	A	496	ASN
1	A	593	ASN
1	B	112	MET
1	B	168	TRP
1	B	186	ASP
1	B	231	LYS
1	B	341	ASN
1	B	344	ASN
1	B	347	GLU
1	B	403	LYS
1	B	408	TRP
1	B	460[A]	GLN
1	B	460[B]	GLN
1	B	462	SER
1	B	593	ASN
1	C	45	ILE
1	C	112	MET
1	C	168	TRP
1	C	185	LYS
1	C	269	ASP
1	C	341	ASN
1	C	385	THR
1	C	400	SER
1	C	408	TRP
1	C	462	SER
1	C	593	ASN
1	D	45	ILE
1	D	112	MET
1	D	168	TRP
1	D	185	LYS
1	D	206	PHE
1	D	299	HIS
1	D	341	ASN
1	D	344	ASN
1	D	403	LYS
1	D	460	GLN
1	D	462	SER

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Mol	Chain	Res	Type
1	D	490	LYS
1	D	593	ASN
1	D	619	THR

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

Mol	Chain	Res	Type
1	A	263	GLN
1	A	299	HIS
1	A	341	ASN
1	A	461	GLN
1	B	263	GLN
1	B	341	ASN
1	B	611	GLN
1	C	263	GLN
1	C	341	ASN
1	C	460	GLN
1	C	611	GLN
1	D	110	GLN
1	D	299	HIS
1	D	341	ASN
1	D	344	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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

16 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	FDA	A	801	1	48,58,58	1.33	4 (8%)	54,89,89	4.66	17 (31%)
3	G2F	A	802	-	11,12,12	1.34	3 (27%)	15,17,17	3.16	6 (40%)
4	1PE	A	803	-	11,11,15	0.78	0	10,10,14	0.57	0
5	MES	A	804	-	11,12,12	0.78	0	14,16,16	2.34	6 (42%)
5	MES	B	701	-	11,12,12	1.24	1 (9%)	14,16,16	1.57	5 (35%)
2	FDA	B	702	1	48,58,58	1.54	11 (22%)	54,89,89	4.74	16 (29%)
3	G2F	B	703	-	11,12,12	1.62	3 (27%)	15,17,17	3.21	10 (66%)
4	1PE	B	704	-	15,15,15	0.60	0	14,14,14	0.42	0
2	FDA	C	801	1	48,58,58	1.37	8 (16%)	54,89,89	3.48	14 (25%)
3	G2F	C	802	-	11,12,12	1.32	1 (9%)	15,17,17	3.12	7 (46%)
4	1PE	C	803	-	15,15,15	0.57	0	14,14,14	0.19	0
2	FDA	D	801	1	48,58,58	1.22	6 (12%)	54,89,89	3.53	18 (33%)
3	G2F	D	802	-	11,12,12	1.13	0	15,17,17	3.91	8 (53%)
4	1PE	D	803	-	15,15,15	0.64	0	14,14,14	0.31	0
5	MES	D	804	-	11,12,12	2.00	6 (54%)	14,16,16	4.91	5 (35%)
5	MES	D	805	-	11,12,12	1.02	1 (9%)	14,16,16	1.47	4 (28%)

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	FDA	A	801	1	-	0/30/50/50	0/6/6/6
3	G2F	A	802	-	-	0/2/22/22	0/1/1/1
4	1PE	A	803	-	-	0/9/9/13	0/0/0/0
5	MES	A	804	-	-	0/6/14/14	0/1/1/1
5	MES	B	701	-	-	0/6/14/14	0/1/1/1
2	FDA	B	702	1	-	0/30/50/50	0/6/6/6
3	G2F	B	703	-	-	0/2/22/22	0/1/1/1
4	1PE	B	704	-	-	0/13/13/13	0/0/0/0
2	FDA	C	801	1	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G2F	C	802	-	-	0/2/22/22	0/1/1/1
4	1PE	C	803	-	-	0/13/13/13	0/0/0/0
2	FDA	D	801	1	-	0/30/50/50	0/6/6/6
3	G2F	D	802	-	-	0/2/22/22	0/1/1/1
4	1PE	D	803	-	-	0/13/13/13	0/0/0/0
5	MES	D	804	-	-	0/6/14/14	0/1/1/1
5	MES	D	805	-	-	0/6/14/14	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	G2F	C2-C3	-3.82	1.48	1.52
2	D	801	FDA	O4B-C4B	-3.44	1.37	1.45
2	A	801	FDA	O4B-C4B	-2.85	1.38	1.45
2	C	801	FDA	O4B-C4B	-2.64	1.38	1.45
2	A	801	FDA	C5A-C4A	-2.51	1.34	1.40
2	B	702	FDA	O4B-C4B	-2.43	1.39	1.45
2	C	801	FDA	O4B-C1B	-2.36	1.38	1.41
2	C	801	FDA	O3B-C3B	-2.33	1.37	1.43
3	B	703	G2F	O4-C4	-2.27	1.37	1.43
3	A	802	G2F	C2-C3	-2.21	1.50	1.52
2	D	801	FDA	O2B-C2B	-2.16	1.37	1.43
2	C	801	FDA	C2B-C3B	-2.13	1.47	1.53
2	C	801	FDA	O4'-C4'	-2.03	1.38	1.43
5	B	701	MES	C3-N4	2.05	1.52	1.46
2	C	801	FDA	C9-C8	2.06	1.43	1.37
2	B	702	FDA	C4-N3	2.07	1.36	1.33
5	D	804	MES	C5-N4	2.08	1.52	1.46
5	D	805	MES	C3-N4	2.10	1.52	1.46
3	A	802	G2F	C4-C3	2.11	1.57	1.52
5	D	804	MES	O1S-S	2.13	1.51	1.45
2	D	801	FDA	C9-C8	2.18	1.43	1.37
5	D	804	MES	O3S-S	2.21	1.52	1.46
3	A	802	G2F	C4-C5	2.25	1.57	1.53
2	B	702	FDA	C8M-C8	2.30	1.55	1.51
2	D	801	FDA	O4B-C1B	2.38	1.44	1.41
2	D	801	FDA	C9A-N10	2.38	1.42	1.38
2	B	702	FDA	C2A-N1A	2.40	1.38	1.33
3	B	703	G2F	O1-C1	2.43	1.48	1.39
2	B	702	FDA	C5X-N5	2.49	1.39	1.35
3	B	703	G2F	C2-C3	2.56	1.54	1.52
2	B	702	FDA	C1'-N10	2.62	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	804	MES	C7-C8	2.67	1.61	1.52
2	B	702	FDA	C9-C8	2.71	1.45	1.37
2	B	702	FDA	C10-N1	2.71	1.40	1.35
5	D	804	MES	C7-N4	2.82	1.54	1.47
2	B	702	FDA	C4-C4X	2.84	1.46	1.41
5	D	804	MES	C3-N4	2.97	1.55	1.46
2	C	801	FDA	C1'-N10	3.01	1.51	1.48
2	A	801	FDA	C10-N1	3.03	1.40	1.35
2	C	801	FDA	C4-C4X	3.33	1.47	1.41
2	D	801	FDA	C4-C4X	3.48	1.48	1.41
2	B	702	FDA	C2A-N3A	3.85	1.39	1.32
2	B	702	FDA	C5'-C4'	3.95	1.57	1.51
2	A	801	FDA	C4-C4X	4.40	1.50	1.41

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FDA	N3A-C2A-N1A	-16.00	116.65	128.89
2	C	801	FDA	C4-C4X-C10	-13.96	111.01	119.94
2	D	801	FDA	N3A-C2A-N1A	-13.53	118.54	128.89
2	C	801	FDA	N3A-C2A-N1A	-13.04	118.91	128.89
2	B	702	FDA	N3A-C2A-N1A	-11.80	119.86	128.89
2	A	801	FDA	C4X-C4-N3	-10.28	109.53	123.59
2	D	801	FDA	C4X-C4-N3	-9.65	110.40	123.59
2	B	702	FDA	C4X-C4-N3	-9.28	110.91	123.59
2	B	702	FDA	C4-C4X-C10	-8.76	114.34	119.94
3	A	802	G2F	O1-C1-O5	-6.25	93.16	110.25
2	A	801	FDA	C4X-C10-N10	-5.94	117.02	120.52
2	B	702	FDA	C4X-C10-N10	-5.79	117.11	120.52
3	B	703	G2F	O1-C1-O5	-4.45	98.09	110.25
2	A	801	FDA	C4-C4X-C10	-4.28	117.20	119.94
2	C	801	FDA	C4B-O4B-C1B	-3.75	105.59	109.72
3	A	802	G2F	F2-C2-C3	-3.38	106.13	108.52
5	D	804	MES	O3S-S-O2S	-3.28	103.97	111.61
2	B	702	FDA	C4B-O4B-C1B	-3.08	106.34	109.72
3	C	802	G2F	O1-C1-O5	-2.97	102.12	110.25
2	D	801	FDA	C4A-C5A-N7A	-2.89	106.82	109.48
2	A	801	FDA	C7-C6-C5X	-2.88	116.22	120.92
2	A	801	FDA	C9A-C5X-N5	-2.78	118.24	122.36
2	D	801	FDA	O4'-C4'-C5'	-2.75	104.20	110.19
2	D	801	FDA	C5X-C9A-N10	-2.72	115.56	117.62
2	B	702	FDA	C4A-C5A-N7A	-2.68	107.02	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	FDA	C8M-C8-C7	-2.51	115.22	120.73
3	D	802	G2F	O1-C1-O5	-2.49	103.43	110.25
5	D	805	MES	O3S-S-O2S	-2.40	106.01	111.61
2	D	801	FDA	C9A-C5X-N5	-2.34	118.89	122.36
5	B	701	MES	O2S-S-O1S	-2.24	105.32	113.48
5	B	701	MES	O3S-S-O2S	-2.21	106.46	111.61
5	A	804	MES	O3S-S-O2S	-2.18	106.53	111.61
5	D	805	MES	O3S-S-O1S	-2.00	106.95	111.61
5	B	701	MES	C2-C3-N4	2.07	113.26	110.12
2	A	801	FDA	C6-C5X-C9A	2.08	121.72	118.98
2	C	801	FDA	C5B-C4B-C3B	2.11	123.60	115.21
3	A	802	G2F	O4-C4-C3	2.12	115.11	110.34
3	B	703	G2F	O5-C1-C2	2.17	118.00	110.46
2	A	801	FDA	O4B-C4B-C3B	2.20	109.59	105.15
2	A	801	FDA	O4B-C4B-C5B	2.24	117.33	109.32
5	D	805	MES	C6-C5-N4	2.32	113.65	110.12
2	B	702	FDA	O4B-C4B-C5B	2.41	117.94	109.32
3	B	703	G2F	O3-C3-C2	2.43	113.38	109.05
5	A	804	MES	O1S-S-C8	2.43	108.98	106.91
2	D	801	FDA	O2'-C2'-C3'	2.44	115.14	109.02
2	D	801	FDA	O4'-C4'-C3'	2.48	115.26	109.02
3	D	802	G2F	O5-C1-C2	2.49	119.12	110.46
5	B	701	MES	O2S-S-C8	2.54	109.07	106.91
2	C	801	FDA	O4B-C4B-C5B	2.57	118.51	109.32
5	B	701	MES	O1S-S-C8	2.59	109.11	106.91
2	B	702	FDA	O4B-C1B-N9A	2.63	113.60	108.10
3	B	703	G2F	C6-C5-C4	2.63	119.50	113.02
5	D	804	MES	C7-N4-C3	2.63	118.02	111.27
2	B	702	FDA	C5B-C4B-C3B	2.64	125.68	115.21
3	D	802	G2F	C6-C5-C4	2.66	119.59	113.02
3	B	703	G2F	O3-C3-C4	2.70	116.42	110.34
2	A	801	FDA	C2A-N1A-C6A	2.75	123.67	118.77
5	D	805	MES	O1S-S-C8	2.76	109.26	106.91
2	C	801	FDA	C2A-N1A-C6A	2.76	123.70	118.77
3	C	802	G2F	O5-C1-C2	2.90	120.54	110.46
5	D	804	MES	C7-C8-S	2.92	121.56	112.51
5	A	804	MES	C6-O1-C2	2.94	119.80	109.89
3	C	802	G2F	O5-C5-C4	2.97	115.25	109.68
5	A	804	MES	O1-C2-C3	2.97	118.64	111.84
2	D	801	FDA	C1'-N10-C9A	3.10	122.34	118.86
2	C	801	FDA	O4B-C4B-C3B	3.17	111.53	105.15
2	B	702	FDA	C1'-N10-C9A	3.19	122.44	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	FDA	C4-C4X-N5	3.19	122.59	118.72
2	D	801	FDA	O4B-C4B-C5B	3.25	120.93	109.32
2	B	702	FDA	O4B-C4B-C3B	3.28	111.75	105.15
2	D	801	FDA	C2A-N1A-C6A	3.29	124.64	118.77
5	A	804	MES	C2-C3-N4	3.35	115.20	110.12
2	D	801	FDA	O2B-C2B-C3B	3.39	122.84	111.83
3	A	802	G2F	O5-C1-C2	3.47	122.50	110.46
2	D	801	FDA	C5B-C4B-C3B	3.48	129.03	115.21
5	D	804	MES	C2-C3-N4	3.49	115.41	110.12
2	A	801	FDA	O2B-C2B-C3B	3.69	123.83	111.83
3	D	802	G2F	O3-C3-C4	3.71	118.70	110.34
2	A	801	FDA	C4X-N5-C5X	3.71	121.04	116.76
3	D	802	G2F	O5-C5-C4	3.75	116.72	109.68
2	B	702	FDA	O2B-C2B-C3B	3.77	124.08	111.83
3	B	703	G2F	O5-C5-C4	3.82	116.85	109.68
2	C	801	FDA	O2B-C2B-C3B	3.87	124.42	111.83
3	A	802	G2F	C1-O5-C5	4.12	121.10	113.47
2	A	801	FDA	O3B-C3B-C4B	4.18	123.58	111.05
3	C	802	G2F	C3-C4-C5	4.37	117.81	110.20
3	B	703	G2F	F2-C2-C3	4.52	111.73	108.52
3	B	703	G2F	C3-C4-C5	4.60	118.22	110.20
3	C	802	G2F	O3-C3-C4	4.65	120.80	110.34
3	B	703	G2F	C1-O5-C5	4.67	122.11	113.47
3	D	802	G2F	C3-C4-C5	4.69	118.36	110.20
2	A	801	FDA	O4B-C1B-N9A	4.71	117.95	108.10
3	C	802	G2F	C1-O5-C5	4.77	122.29	113.47
2	C	801	FDA	C1'-N10-C9A	4.84	124.29	118.86
2	C	801	FDA	C4-C4X-N5	4.88	124.64	118.72
2	D	801	FDA	O4B-C1B-N9A	4.88	118.32	108.10
5	A	804	MES	O2S-S-C8	4.97	111.14	106.91
2	C	801	FDA	O3B-C3B-C4B	5.07	126.27	111.05
2	A	801	FDA	C1'-N10-C9A	5.17	124.67	118.86
2	D	801	FDA	C4X-N5-C5X	5.19	122.73	116.76
3	B	703	G2F	F2-C2-C1	5.21	115.94	108.59
2	C	801	FDA	O4B-C1B-N9A	5.44	119.50	108.10
2	D	801	FDA	O3B-C3B-C4B	5.61	127.89	111.05
3	D	802	G2F	C1-O5-C5	5.96	124.50	113.47
3	C	802	G2F	F2-C2-C1	6.76	118.13	108.59
2	C	801	FDA	C4-N3-C2	6.83	121.15	115.25
3	A	802	G2F	F2-C2-C1	7.01	118.48	108.59
2	D	801	FDA	C2B-C1B-N9A	7.17	125.24	114.29
2	C	801	FDA	C2B-C1B-N9A	7.37	125.55	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FDA	C2B-C1B-N9A	7.86	126.31	114.29
2	B	702	FDA	C2B-C1B-N9A	8.21	126.83	114.29
3	D	802	G2F	F2-C2-C3	10.80	116.18	108.52
2	D	801	FDA	C4-N3-C2	12.08	125.69	115.25
5	D	804	MES	O2S-S-C8	17.14	121.53	106.91
2	A	801	FDA	C4-N3-C2	22.85	135.00	115.25
2	B	702	FDA	C4-N3-C2	26.24	137.94	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	701	MES	1	0
2	B	702	FDA	2	0
3	B	703	G2F	1	0
2	C	801	FDA	2	0
3	C	802	G2F	1	0
2	D	801	FDA	2	0
3	D	802	G2F	1	0
4	D	803	1PE	4	0
5	D	804	MES	9	0
5	D	805	MES	1	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	576/633 (90%)	-0.31	17 (2%) 54 55	17, 23, 45, 78	0
1	B	576/633 (90%)	-0.33	10 (1%) 73 73	16, 22, 39, 68	1 (0%)
1	C	574/633 (90%)	-0.06	19 (3%) 50 51	20, 34, 54, 81	0
1	D	575/633 (90%)	-0.23	11 (1%) 70 70	18, 27, 47, 74	0
All	All	2301/2532 (90%)	-0.23	57 (2%) 61 61	16, 26, 48, 81	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	618	PHE	7.6
1	D	389	LEU	6.7
1	B	618	PHE	5.9
1	D	343	ALA	5.3
1	C	343	ALA	4.8
1	C	270	ALA	4.8
1	A	389	LEU	4.6
1	A	388	GLU	4.5
1	B	45	ILE	4.5
1	D	385	THR	4.4
1	A	385	THR	4.3
1	D	390	THR	4.3
1	D	345	PRO	3.8
1	A	343	ALA	3.7
1	C	272	GLU	3.6
1	B	343	ALA	3.4
1	C	616	SER	3.3
1	C	617	PRO	3.3
1	B	342	PRO	3.3
1	D	618	PHE	3.3
1	A	391	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	44	ASP	3.2
1	C	68	ALA	3.1
1	C	385	THR	3.0
1	C	344	ASN	3.0
1	A	382	ILE	3.0
1	A	387	GLY	3.0
1	C	266	PRO	3.0
1	A	393	VAL	2.9
1	C	268	THR	2.9
1	C	271	PRO	2.9
1	B	268	THR	2.9
1	C	269	ASP	2.8
1	B	344	ASN	2.8
1	A	618	PHE	2.7
1	B	44	ASP	2.7
1	D	388	GLU	2.7
1	D	383	ARG	2.5
1	A	344	ASN	2.4
1	D	344	ASN	2.4
1	C	267	ASN	2.4
1	B	460[A]	GLN	2.4
1	C	274	ARG	2.4
1	A	268	THR	2.4
1	B	385	THR	2.3
1	A	390	THR	2.3
1	A	45	ILE	2.2
1	A	272	GLU	2.2
1	B	389	LEU	2.2
1	D	387	GLY	2.2
1	A	401	THR	2.1
1	C	66	VAL	2.1
1	A	269	ASP	2.1
1	D	560	LYS	2.1
1	C	345	PRO	2.1
1	C	65	LEU	2.0
1	C	70	TYR	2.0

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

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

### 6.3 Carbohydrates [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
5	MES	A	804	12/12	0.81	0.25	5.72	69,76,94,113	0
5	MES	D	804	12/12	0.85	0.24	3.69	35,44,54,54	0
4	1PE	B	704	16/16	0.90	0.15	3.35	34,38,52,54	0
5	MES	B	701	12/12	0.96	0.15	2.58	31,37,43,44	0
4	1PE	C	803	16/16	0.91	0.18	2.13	43,47,57,57	0
4	1PE	D	803	16/16	0.91	0.15	1.97	37,40,54,55	0
4	1PE	A	803	12/16	0.90	0.11	1.44	30,36,39,40	0
5	MES	D	805	12/12	0.97	0.15	1.24	31,33,40,41	0
3	G2F	D	802	12/12	0.95	0.12	0.38	27,30,31,34	0
3	G2F	C	802	12/12	0.94	0.11	0.27	31,37,40,43	0
3	G2F	A	802	12/12	0.95	0.10	0.10	24,27,29,29	0
2	FDA	A	801	53/53	0.98	0.09	-0.34	16,19,20,23	0
3	G2F	B	703	12/12	0.96	0.10	-0.58	23,25,27,32	0
2	FDA	D	801	53/53	0.98	0.08	-0.61	19,22,27,29	0
2	FDA	B	702	53/53	0.98	0.09	-0.62	13,17,20,21	0
2	FDA	C	801	53/53	0.97	0.08	-0.66	23,27,30,32	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.