W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 8, 2017 – 06:41 PM EST

PDB ID	:	4MOE
Title	:	Pyranose 2-oxidase H450G mutant with 3-fluorinated glucose
Authors	:	Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on	:	unknown
Resolution	:	2.00 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*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

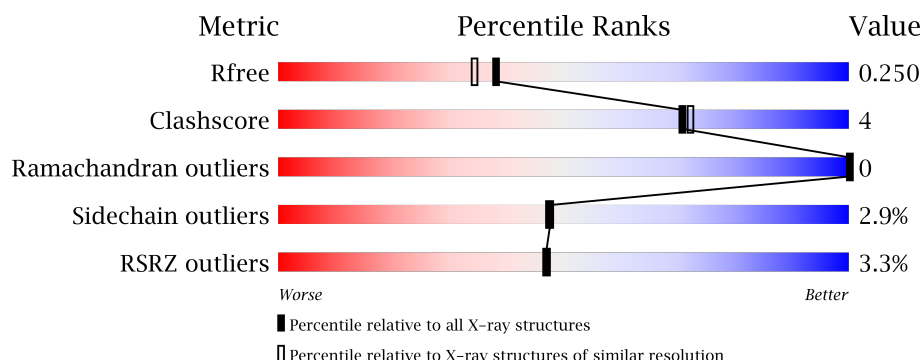|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.250
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.9%
RSRZ outliers		3.3%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 >=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 <=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% — 82% — 8% • 9%
1	B	633	.% — 79% — 11% • 9%
1	C	633	4% — 78% — 12% 9%
1	D	633	4% — 80% — 10% • 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	12P	A	803	-	-	-	X
4	12P	B	803	-	-	-	X
5	MES	A	804	-	-	X	X
5	MES	B	804	-	-	-	X
5	MES	C	803	-	-	-	X
5	MES	D	804	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 19611 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
			4536	2864	775	872	25			
1	B	576	Total	C	N	O	S	0	0	0
			4536	2864	775	872	25			
1	C	574	Total	C	N	O	S	0	0	0
			4520	2855	773	868	24			
1	D	575	Total	C	N	O	S	0	0	0
			4527	2859	774	870	24			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
A	450	GLY	HIS	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	SEE REMARK 999	UNP Q7ZA32
B	450	GLY	HIS	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
B	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
B	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32

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Chain	Residue	Modelled	Actual	Comment	Reference
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	SEE REMARK 999	UNP Q7ZA32
C	450	GLY	HIS	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	SEE REMARK 999	UNP Q7ZA32
D	450	GLY	HIS	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: $C_{27}H_{35}N_9O_{15}P_2$).
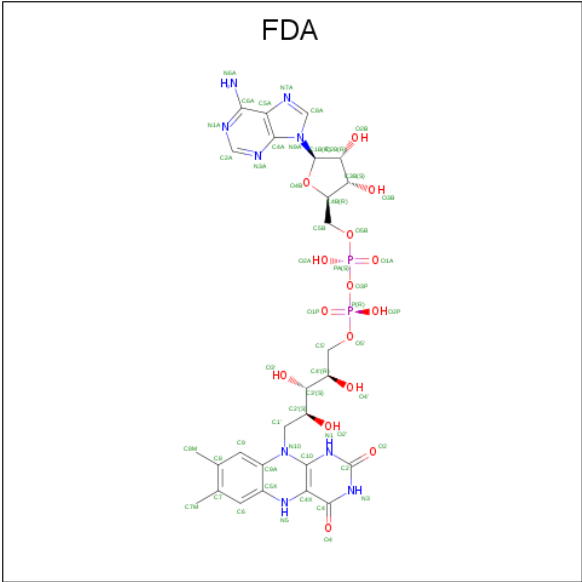
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-deoxy-3-fluoro-beta-D-glucopyranose (three-letter code: G3F) (formula: $C_6H_{11}FO_5$).
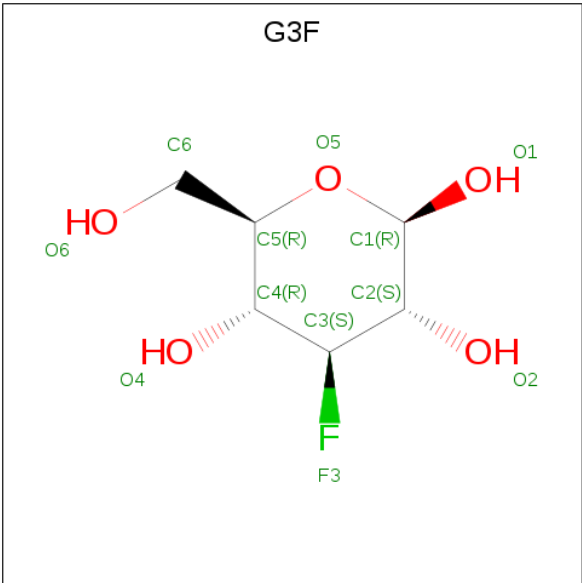
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 6	F 1	O 5	0	0
3	B	1	Total 12	C 6	F 1	O 5	0	0
3	C	1	Total 12	C 6	F 1	O 5	0	0
3	D	1	Total 12	C 6	F 1	O 5	0	0

- Molecule 4 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: $C_{24}H_{50}O_{13}$).
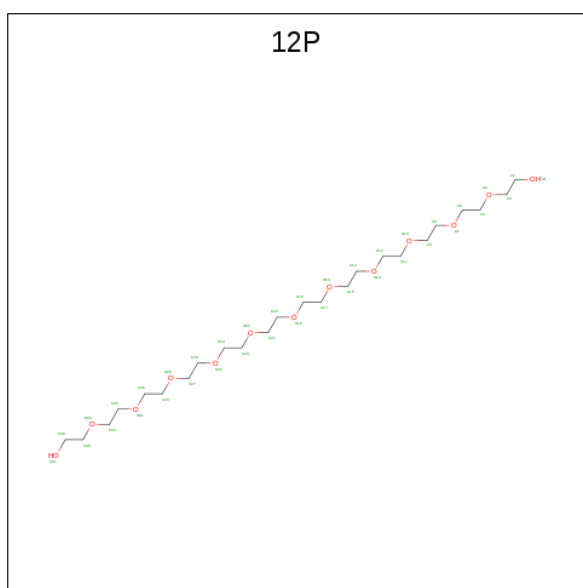
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 15	C 10	O 5	0	0
4	A	1	Total 14	C 9	O 5	0	0
4	B	1	Total 16	C 10	O 6	0	0
4	B	1	Total 11	C 8	O 3	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

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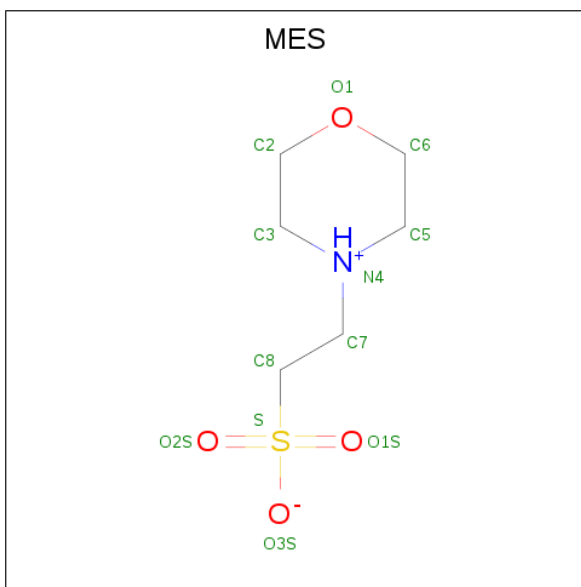
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 12	C 6	N 1	O 4	S 1	0	0
5	B	1	Total 12	C 6	N 1	O 4	S 1	0	0
5	C	1	Total 12	C 6	N 1	O 4	S 1	0	0
5	D	1	Total 12	C 6	N 1	O 4	S 1	0	0
5	D	1	Total 12	C 6	N 1	O 4	S 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	294	Total 294	O 294	0	0
6	B	369	Total 369	O 369	0	0
6	C	183	Total 183	O 183	0	0
6	D	270	Total 270	O 270	0	0

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 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.
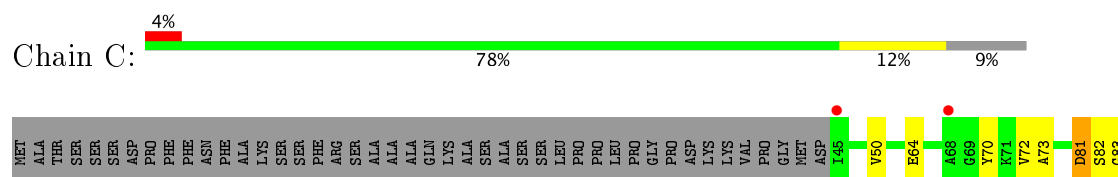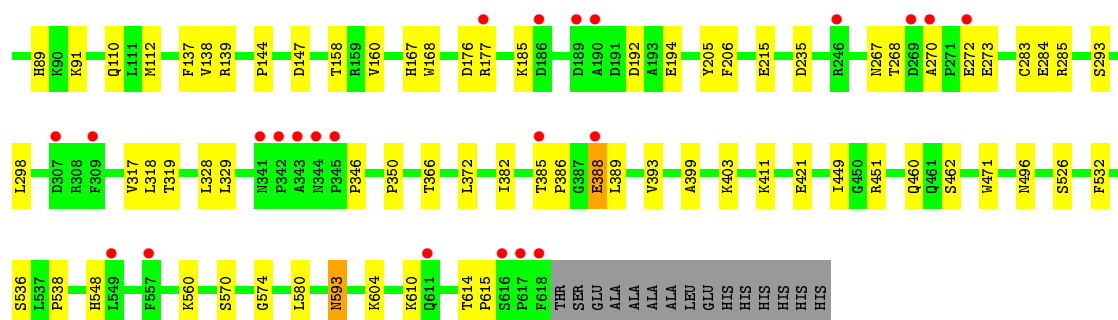
- Molecule 1: Pyranose 2-oxidase
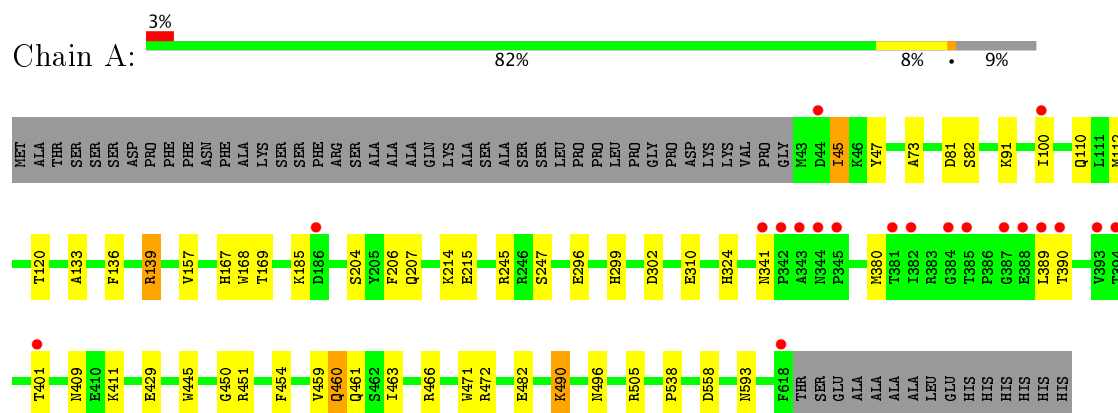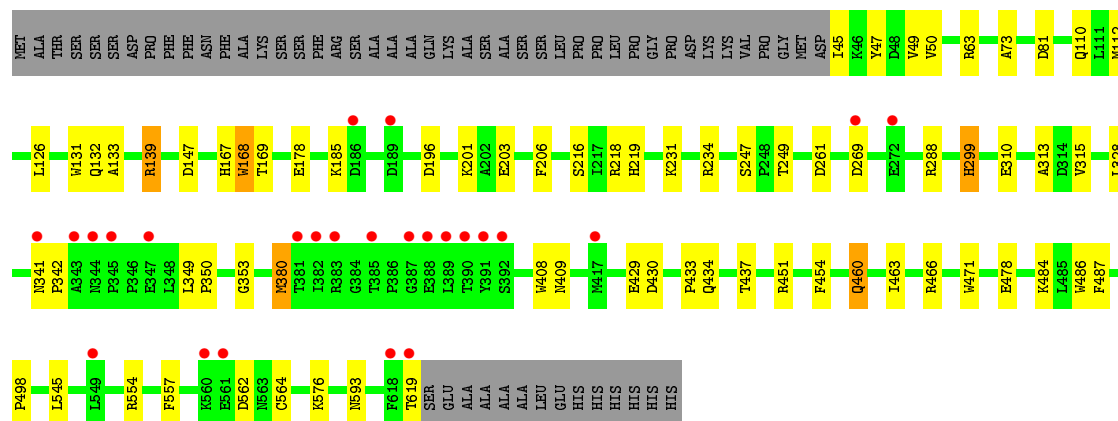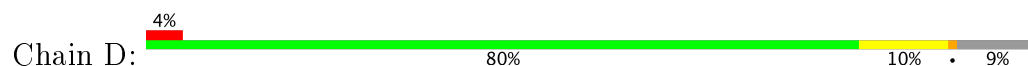

- Molecule 1: Pyranose 2-oxidase

- Molecule 1: Pyranose 2-oxidase

• **Molecule 1: Pyranose 2-oxidase**

Chain D:
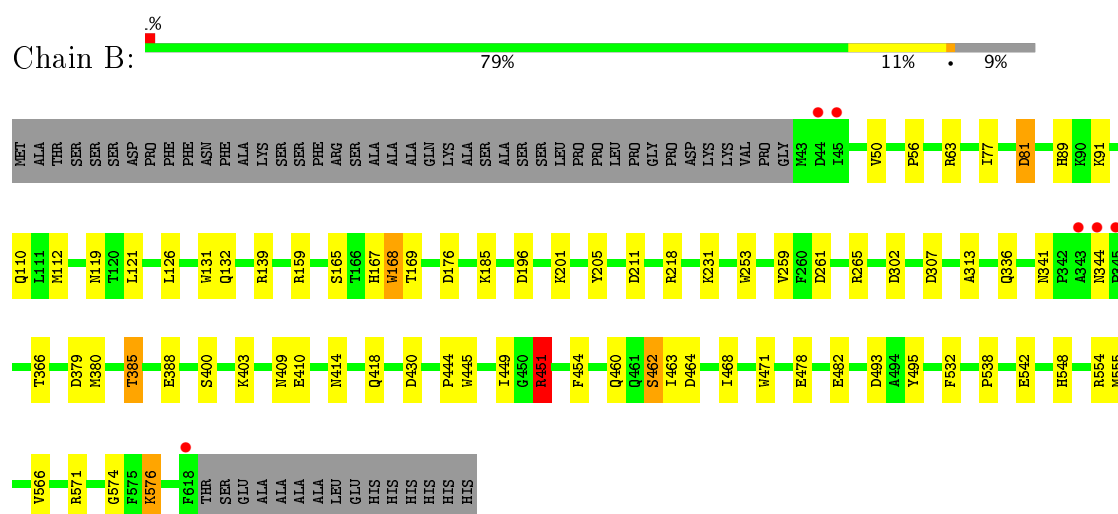
4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.07Å　　102.74Å　　137.69Å 90.00°　　90.80°　　90.00°	Depositor
Resolution (Å)	50.00　–　2.00 41.94　–　2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.00) 97.8 (41.94-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.32 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195　,　0.242 0.202　,　0.250	Depositor DCC
R_{free} test set	3287 reflections (1.82%)	DCC
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.5	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l 0.022 for k,h,-l 0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19611	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: FDA, 12P, MES, G3F

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	1.07	5/4651 (0.1%)	1.02	10/6323 (0.2%)
1	B	1.14	8/4651 (0.2%)	1.07	21/6323 (0.3%)
1	C	0.89	3/4635 (0.1%)	0.89	6/6302 (0.1%)
1	D	1.02	6/4642 (0.1%)	0.98	13/6312 (0.2%)
All	All	1.04	22/18579 (0.1%)	0.99	50/25260 (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

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	TRP	CD2-CE2	7.54	1.50	1.41
1	A	445	TRP	CD2-CE2	7.07	1.49	1.41
1	B	482	GLU	CD-OE1	6.83	1.33	1.25
1	B	478	GLU	CD-OE1	6.54	1.32	1.25
1	A	471	TRP	CD2-CE2	6.11	1.48	1.41

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	B	139	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	C	147	ASP	CB-CG-OD1	9.98	127.29	118.30
1	D	139	ARG	NE-CZ-NH1	9.84	125.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	ARG	NE-CZ-NH2	-9.45	115.57	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4536	0	4384	28	0
1	B	4536	0	4384	37	0
1	C	4520	0	4371	47	0
1	D	4527	0	4378	30	0
2	A	53	0	30	2	0
2	B	53	0	30	2	0
2	C	53	0	29	3	0
2	D	53	0	30	3	0
3	A	12	0	11	1	0
3	B	12	0	11	2	0
3	C	12	0	11	3	0
3	D	12	0	11	2	0
4	A	29	0	34	0	0
4	B	27	0	33	0	0
5	A	12	0	13	10	0
5	B	12	0	13	0	0
5	C	12	0	13	1	0
5	D	24	0	26	1	0
6	A	294	0	0	1	0
6	B	369	0	0	3	0
6	C	183	0	0	1	0
6	D	270	0	0	2	0
All	All	19611	0	17812	147	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.

The worst 5 of 147 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:A:133:ALA:CB	5:A:804:MES:H71	1.53	1.35
1:A:133:ALA:HB3	5:A:804:MES:H71	1.16	1.14
1:A:133:ALA:HB2	5:A:804:MES:H71	1.40	1.00
1:A:133:ALA:CB	5:A:804:MES:C7	2.46	0.92
1:D:460:GLN:HE22	1:D:463:ILE:H	1.13	0.92

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	574/633 (91%)	560 (98%)	14 (2%)	0	100	100
1	B	574/633 (91%)	558 (97%)	16 (3%)	0	100	100
1	C	572/633 (90%)	551 (96%)	21 (4%)	0	100	100
1	D	573/633 (90%)	556 (97%)	17 (3%)	0	100	100
All	All	2293/2532 (91%)	2225 (97%)	68 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	485 (96%)	18 (4%)	40	38
1	B	503/547 (92%)	490 (97%)	13 (3%)	51	52
1	C	501/547 (92%)	489 (98%)	12 (2%)	54	56
1	D	502/547 (92%)	486 (97%)	16 (3%)	44	42
All	All	2009/2188 (92%)	1950 (97%)	59 (3%)	48	47

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	451	ARG
1	C	168	TRP
1	D	454	PHE
1	B	454	PHE
1	B	462	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	563	ASN
1	C	105	ASN
1	D	299	HIS
1	B	344	ASN
1	D	341	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

17 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	51,58,58	1.70	7 (13%)	54,89,89	5.18	20 (37%)
3	G3F	A	802	-	12,12,12	1.42	2 (16%)	14,17,17	1.63	4 (28%)
4	12P	A	803	-	14,14,36	0.73	0	13,13,35	1.10	1 (7%)
5	MES	A	804	-	12,12,12	1.97	2 (16%)	14,16,16	4.05	8 (57%)
4	12P	A	805	-	13,13,36	0.69	0	12,12,35	0.48	0
2	FDA	B	801	1	51,58,58	1.65	12 (23%)	54,89,89	4.73	21 (38%)
3	G3F	B	802	-	12,12,12	1.10	1 (8%)	14,17,17	3.87	4 (28%)
4	12P	B	803	-	15,15,36	0.51	0	14,14,35	0.67	0
5	MES	B	804	-	12,12,12	1.68	1 (8%)	14,16,16	2.03	5 (35%)
4	12P	B	805	-	10,10,36	0.83	0	9,9,35	0.87	0
2	FDA	C	801	1	51,58,58	1.50	11 (21%)	54,89,89	2.97	20 (37%)
3	G3F	C	802	-	12,12,12	1.39	1 (8%)	14,17,17	1.75	4 (28%)
5	MES	C	803	-	12,12,12	2.15	1 (8%)	14,16,16	2.09	2 (14%)
2	FDA	D	801	1	51,58,58	1.51	8 (15%)	54,89,89	4.19	15 (27%)
3	G3F	D	802	-	12,12,12	0.90	0	14,17,17	1.76	2 (14%)
5	MES	D	803	-	12,12,12	1.88	2 (16%)	14,16,16	4.41	3 (21%)
5	MES	D	804	-	12,12,12	1.97	1 (8%)	14,16,16	2.79	5 (35%)

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	-	0/28/50/50	0/6/6/6
3	G3F	A	802	-	-	0/2/22/22	0/1/1/1
4	12P	A	803	-	-	0/12/12/34	0/0/0/0
5	MES	A	804	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	12P	A	805	-	-	0/11/11/34	0/0/0/0
2	FDA	B	801	1	-	0/28/50/50	0/6/6/6
3	G3F	B	802	-	-	0/2/22/22	0/1/1/1
4	12P	B	803	-	-	0/13/13/34	0/0/0/0
5	MES	B	804	-	-	0/6/14/14	0/1/1/1
4	12P	B	805	-	-	0/8/8/34	0/0/0/0
2	FDA	C	801	1	-	0/28/50/50	0/6/6/6
3	G3F	C	802	-	-	0/2/22/22	0/1/1/1
5	MES	C	803	-	-	0/6/14/14	0/1/1/1
2	FDA	D	801	1	-	0/28/50/50	0/6/6/6
3	G3F	D	802	-	-	0/2/22/22	0/1/1/1
5	MES	D	803	-	-	0/6/14/14	0/1/1/1
5	MES	D	804	-	-	0/6/14/14	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	803	MES	C8-S	-7.01	1.67	1.77
5	D	804	MES	C8-S	-5.97	1.68	1.77
5	A	804	MES	C8-S	-5.53	1.69	1.77
5	D	803	MES	C8-S	-4.96	1.70	1.77
5	B	804	MES	C8-S	-4.85	1.70	1.77

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	FDA	C4X-C4-N3	-15.76	101.04	123.48
2	A	801	FDA	N3A-C2A-N1A	-13.97	116.69	128.86
2	B	801	FDA	C4X-C4-N3	-13.76	103.89	123.48
2	D	801	FDA	C4X-C4-N3	-11.81	106.67	123.48
2	C	801	FDA	C4-C4X-C10	-10.75	111.26	119.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FDA	2	0
3	A	802	G3F	1	0
5	A	804	MES	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	FDA	2	0
3	B	802	G3F	2	0
2	C	801	FDA	3	0
3	C	802	G3F	3	0
5	C	803	MES	1	0
2	D	801	FDA	3	0
3	D	802	G3F	2	0
5	D	803	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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	576/633 (90%)	-0.11	20 (3%)	44	45	12, 19, 43, 72	0
1	B	576/633 (90%)	-0.26	6 (1%)	82	82	11, 18, 34, 59	0
1	C	574/633 (90%)	0.15	25 (4%)	35	35	15, 33, 56, 81	0
1	D	575/633 (90%)	-0.08	25 (4%)	36	36	13, 23, 44, 71	0
All	All	2301/2532 (90%)	-0.07	76 (3%)	47	47	11, 23, 49, 81	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	389	LEU	6.9
1	A	382	ILE	6.1
1	D	343	ALA	5.9
1	D	385	THR	5.9
1	C	343	ALA	5.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
5	MES	A	804	12/12	0.91	0.24	6.45	28,41,47,53	0
5	MES	C	803	12/12	0.59	0.30	4.29	74,83,106,113	0
5	MES	B	804	12/12	0.97	0.16	4.00	27,29,36,36	0
4	12P	A	803	15/37	0.88	0.16	3.49	27,32,45,47	0
4	12P	B	803	16/37	0.93	0.15	3.02	31,34,65,69	0
5	MES	D	804	12/12	0.92	0.20	2.35	31,34,40,40	0
4	12P	B	805	11/37	0.82	0.18	1.46	38,44,46,47	0
5	MES	D	803	12/12	0.97	0.13	1.32	24,30,32,33	0
4	12P	A	805	14/37	0.91	0.13	1.26	27,32,37,39	0
3	G3F	C	802	12/12	0.89	0.14	0.22	29,35,37,38	0
3	G3F	D	802	12/12	0.94	0.12	-0.09	23,24,28,28	0
2	FDA	D	801	53/53	0.97	0.11	-0.23	10,15,21,31	0
2	FDA	A	801	53/53	0.98	0.12	-0.25	6,10,14,17	0
2	FDA	C	801	53/53	0.96	0.12	-0.27	16,24,29,33	0
2	FDA	B	801	53/53	0.98	0.10	-0.37	7,10,14,17	0
3	G3F	A	802	12/12	0.95	0.10	-0.99	20,22,25,26	0
3	G3F	B	802	12/12	0.97	0.08	-2.19	22,24,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.