



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:48 PM GMT

PDB ID : 4MOR
Title : Pyranose 2-oxidase H450G/V546C double mutant with 3-fluorinated galactose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 1.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

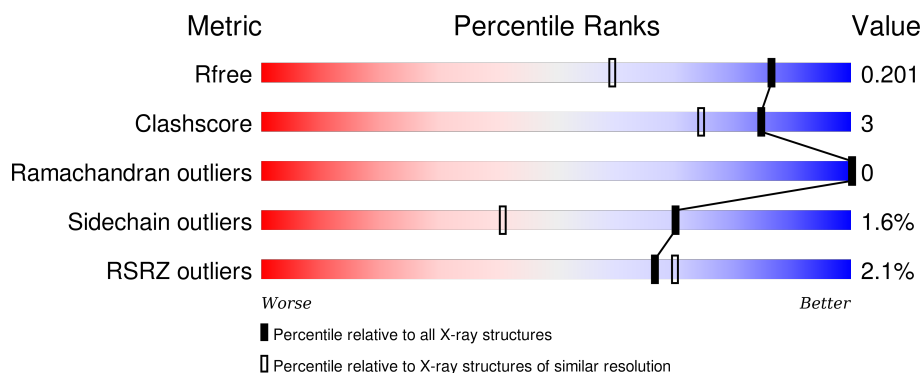
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 $\leq 5\%$. 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	<div> <div>2%</div> <div>81% 10% 9%</div> </div>
1	B	633	<div> <div>2%</div> <div>79% 11% 9%</div> </div>
1	C	633	<div> <div>2%</div> <div>83% 7% 9%</div> </div>
1	D	633	<div> <div>2%</div> <div>83% 7% 9%</div> </div>

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	12P	A	803	-	-	-	X
4	12P	C	803	-	-	-	X
5	MES	B	804	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21660 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	8	0
			4571	2890	775	879	27			
1	B	576	Total	C	N	O	S	0	10	0
			4595	2905	781	882	27			
1	C	573	Total	C	N	O	S	0	4	0
			4531	2862	772	872	25			
1	D	576	Total	C	N	O	S	0	5	0
			4561	2881	775	879	26			

There are 56 discrepancies between the modelled and reference sequences:

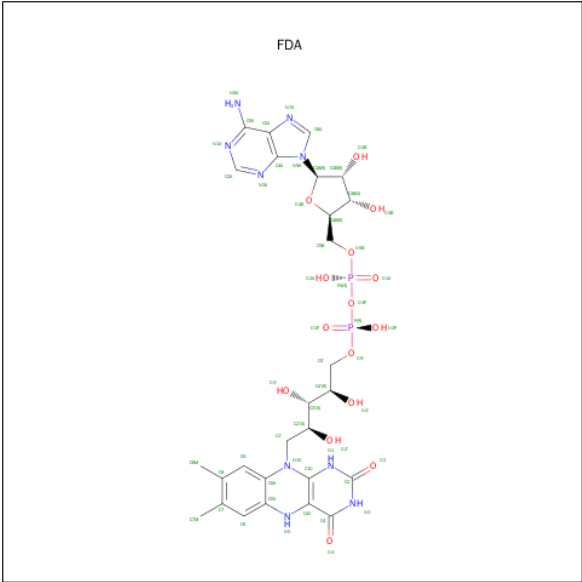
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
A	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
A	546	CYS	VAL	ENGINEERED MUTATION	UNP Q7ZA32
A	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	626	LEU	-	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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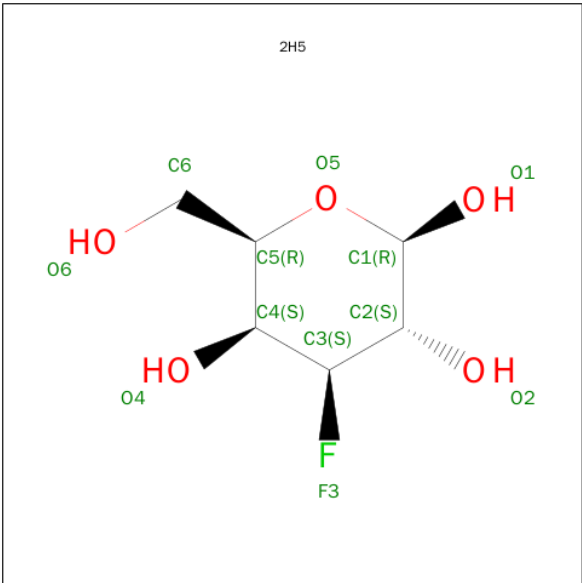
Chain	Residue	Modelled	Actual	Comment	Reference
B	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
B	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	633	HIS	-	EXPRESSION TAG	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: C₂₇H₃₅N₉O₁₅P₂).



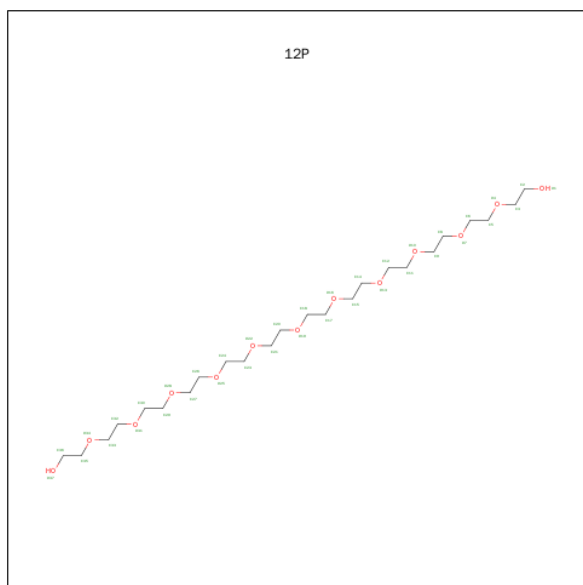
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-DEOXY-3-FLUORO-BETA-D-GALACTOPYRANOSE (three-letter code: 2H5) (formula: C₆H₁₁FO₅).



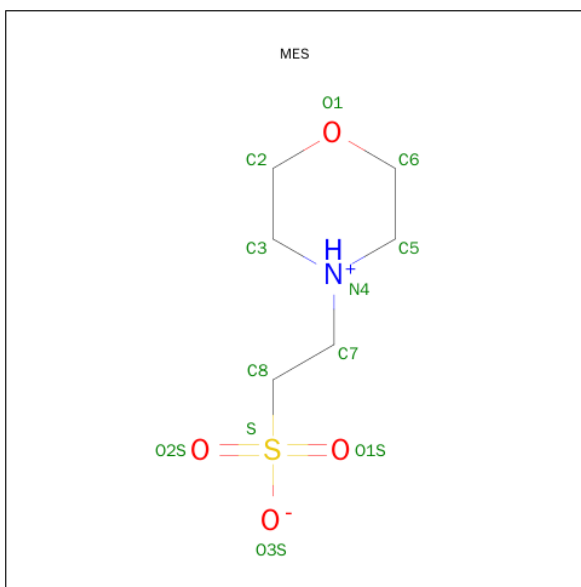
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			12	6	1	5		
3	B	1	Total	C	F	O	0	0
			12	6	1	5		
3	C	1	Total	C	F	O	0	0
			12	6	1	5		
3	D	1	Total	C	F	O	0	0
			12	6	1	5		

- 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	C	O	0	0
			15	10	5		
4	B	1	Total	C	O	0	0
			16	10	6		
4	C	1	Total	C	O	0	0
			11	8	3		
4	D	1	Total	C	O	0	0
			14	9	5		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

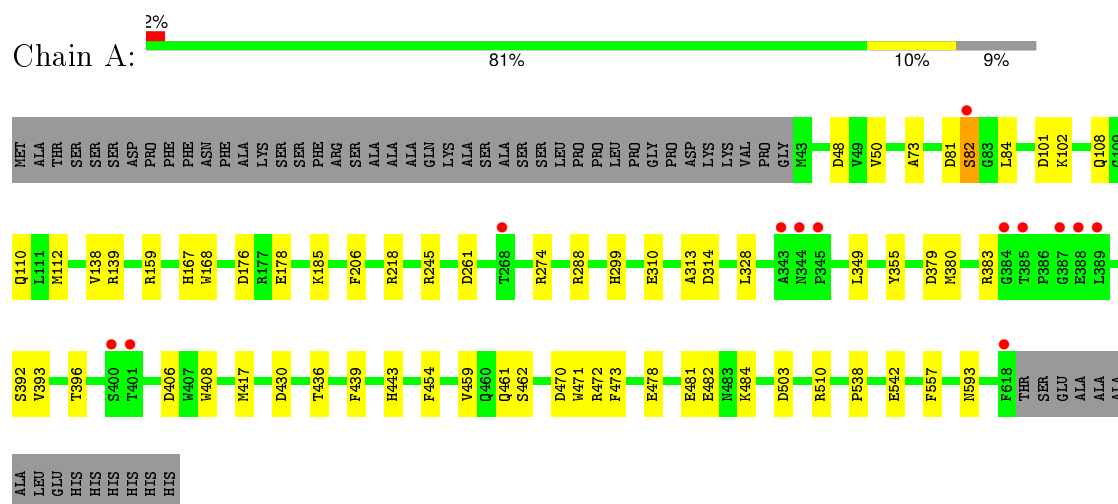
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	839	Total	O	0	0
			839	839		
6	B	847	Total	O	0	0
			847	847		
6	C	653	Total	O	0	0
			653	653		
6	D	723	Total	O	0	0
			723	723		

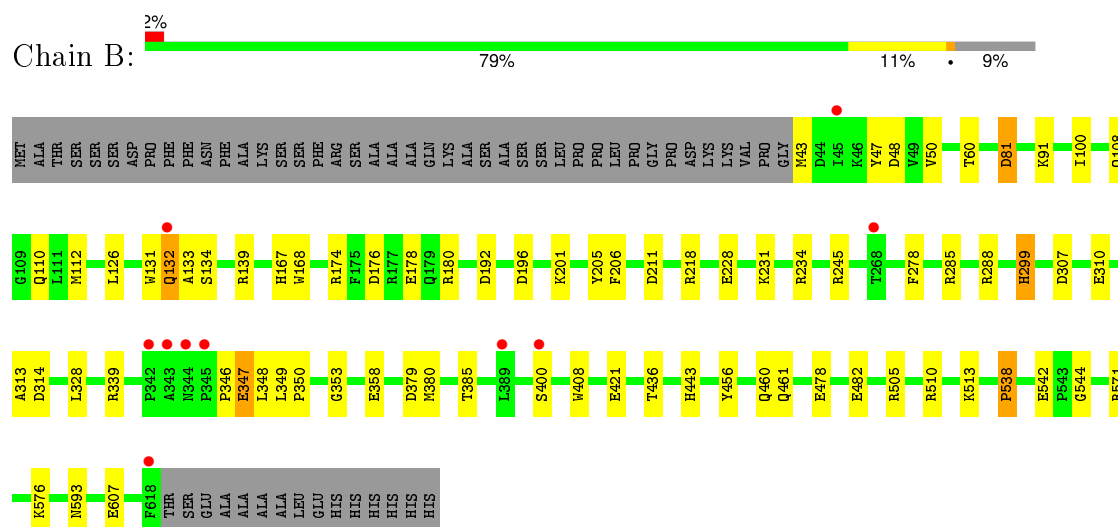
3 Residue-property plots [i](#)

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

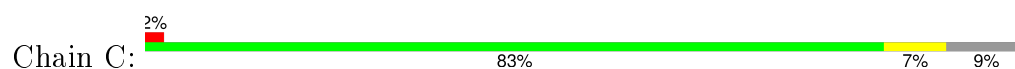
• Molecule 1: Pyranose 2-oxidase

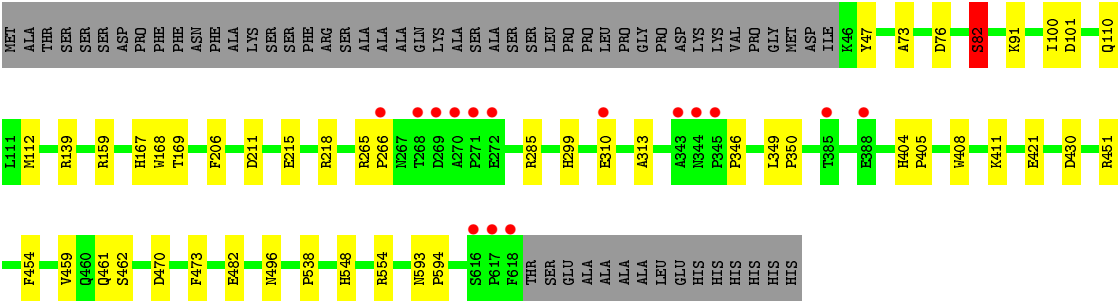


• Molecule 1: Pyranose 2-oxidase

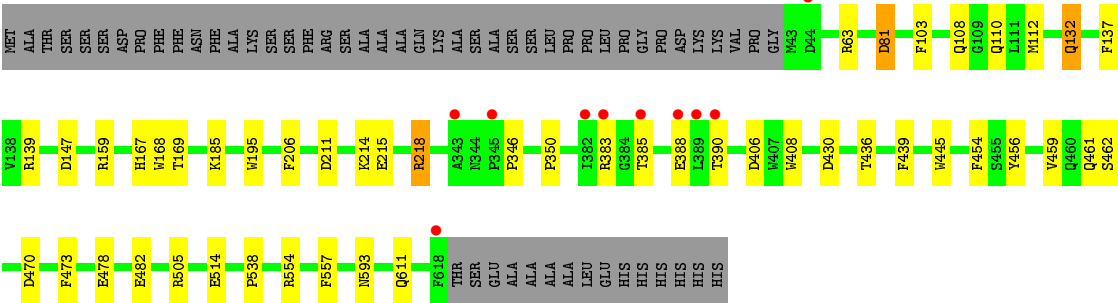
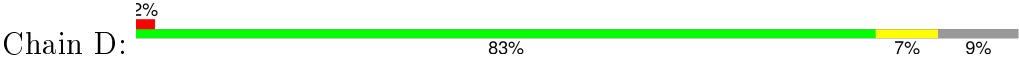


• Molecule 1: Pyranose 2-oxidase





● 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, α , β , γ	100.24Å 102.47Å 137.84Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	49.33 – 1.50 49.33 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.33-1.50) 99.7 (49.33-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.198 0.166 , 0.201	Depositor DCC
R_{free} test set	1107 reflections (0.25%)	DCC
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.9	EDS
Estimated twinning fraction	0.016 for -k,-h,-l 0.012 for k,h,-l 0.022 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 442699 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21660	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 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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, 12P, 2H5, MES

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	1.29	15/4710 (0.3%)	1.20	33/6403 (0.5%)
1	B	1.32	23/4746 (0.5%)	1.30	36/6449 (0.6%)
1	C	1.13	3/4658 (0.1%)	1.04	10/6333 (0.2%)
1	D	1.19	9/4694 (0.2%)	1.13	20/6381 (0.3%)
All	All	1.24	50/18808 (0.3%)	1.17	99/25566 (0.4%)

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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	GLU	CD-OE1	14.32	1.41	1.25
1	B	478	GLU	CD-OE1	14.09	1.41	1.25
1	D	478	GLU	CD-OE2	11.10	1.37	1.25
1	D	482	GLU	CD-OE2	9.25	1.35	1.25
1	A	310	GLU	CD-OE2	8.37	1.34	1.25
1	A	482	GLU	CD-OE1	8.29	1.34	1.25
1	B	400	SER	CB-OG	7.89	1.52	1.42
1	D	132	GLN	C-O	7.66	1.37	1.23
1	B	347	GLU	CD-OE1	7.41	1.33	1.25
1	B	421	GLU	CD-OE2	7.21	1.33	1.25
1	B	139	ARG	CD-NE	-6.90	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	482	GLU	CD-OE1	6.75	1.33	1.25
1	B	299	HIS	CG-CD2	6.55	1.46	1.35
1	B	478	GLU	CG-CD	6.46	1.61	1.51
1	A	478	GLU	CD-OE2	6.35	1.32	1.25
1	B	228	GLU	CD-OE1	6.30	1.32	1.25
1	A	310	GLU	CG-CD	6.09	1.61	1.51
1	D	81	ASP	CB-CG	-6.07	1.39	1.51
1	B	400	SER	CA-CB	6.00	1.61	1.52
1	B	180	ARG	CZ-NH2	-5.99	1.25	1.33
1	D	456	TYR	CE1-CZ	5.96	1.46	1.38
1	B	456	TYR	CE1-CZ	5.89	1.46	1.38
1	A	82	SER	N-CA	5.86	1.58	1.46
1	A	482	GLU	CD-OE2	5.81	1.32	1.25
1	B	542	GLU	CD-OE1	5.78	1.32	1.25
1	A	245	ARG	CZ-NH1	5.72	1.40	1.33
1	D	514	GLU	CD-OE2	5.69	1.31	1.25
1	A	443	HIS	CG-CD2	5.68	1.45	1.35
1	A	482	GLU	CG-CD	5.67	1.60	1.51
1	C	482	GLU	CD-OE1	5.57	1.31	1.25
1	B	132[A]	GLN	C-O	5.56	1.33	1.23
1	B	132[B]	GLN	C-O	5.56	1.33	1.23
1	B	132[C]	GLN	C-O	5.56	1.33	1.23
1	C	462	SER	CB-OG	-5.54	1.35	1.42
1	B	339	ARG	CZ-NH2	5.52	1.40	1.33
1	A	542	GLU	CD-OE2	5.50	1.31	1.25
1	A	355	TYR	CE1-CZ	-5.41	1.31	1.38
1	A	299	HIS	CG-CD2	5.39	1.45	1.35
1	D	478	GLU	CG-CD	5.38	1.60	1.51
1	C	421	GLU	CD-OE1	-5.33	1.19	1.25
1	B	131	TRP	CD2-CE2	5.33	1.47	1.41
1	B	482	GLU	CD-OE1	5.23	1.31	1.25
1	A	471	TRP	CD2-CE2	5.22	1.47	1.41
1	B	542	GLU	CD-OE2	5.17	1.31	1.25
1	B	443	HIS	CG-CD2	5.12	1.44	1.35
1	B	482	GLU	CD-OE2	5.11	1.31	1.25
1	B	353	GLY	C-O	-5.10	1.15	1.23
1	D	195	TRP	CD2-CE2	5.06	1.47	1.41
1	B	81	ASP	CB-CG	-5.05	1.41	1.51
1	A	542	GLU	CD-OE1	5.03	1.31	1.25

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH1	17.70	129.15	120.30
1	B	139	ARG	NE-CZ-NH1	17.50	129.05	120.30
1	B	139	ARG	NE-CZ-NH2	-17.18	111.71	120.30
1	A	139	ARG	NE-CZ-NH1	14.52	127.56	120.30
1	D	139	ARG	NE-CZ-NH2	-13.37	113.62	120.30
1	B	218	ARG	NE-CZ-NH1	12.99	126.80	120.30
1	A	139	ARG	NE-CZ-NH2	-12.65	113.97	120.30
1	B	380	MET	CG-SD-CE	-12.21	80.67	100.20
1	A	218	ARG	NE-CZ-NH1	11.33	125.97	120.30
1	B	81	ASP	CB-CG-OD1	-11.21	108.22	118.30
1	B	211	ASP	CB-CG-OD1	10.94	128.14	118.30
1	B	505	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	B	211	ASP	CB-CG-OD2	-9.35	109.89	118.30
1	C	470	ASP	CB-CG-OD2	-9.18	110.03	118.30
1	D	81	ASP	CB-CG-OD1	-9.05	110.15	118.30
1	A	159	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	D	63	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	472	ARG	NE-CZ-NH2	8.45	124.52	120.30
1	A	82	SER	CB-CA-C	-8.36	94.22	110.10
1	D	211	ASP	CB-CG-OD1	8.27	125.75	118.30
1	D	218	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	307	ASP	CB-CG-OD1	8.03	125.52	118.30
1	B	196	ASP	CB-CG-OD1	7.74	125.27	118.30
1	B	505	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	470	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	234	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	139	ARG	CD-NE-CZ	7.54	134.16	123.60
1	B	314	ASP	CB-CG-OD1	7.46	125.01	118.30
1	C	139	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	C	139	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	406	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	174	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	576	LYS	CD-CE-NZ	7.29	128.47	111.70
1	D	505	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	48	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	211	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	473	PHE	CB-CG-CD1	7.05	125.74	120.80
1	B	349	LEU	CB-CG-CD2	7.05	122.98	111.00
1	A	159	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	314	ASP	CB-CG-OD1	6.85	124.46	118.30
1	C	159	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	380	MET	CG-SD-CE	-6.76	89.38	100.20
1	A	379	ASP	CB-CG-OD2	-6.76	112.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	A	84	LEU	CB-CG-CD1	-6.61	99.76	111.00
1	B	81	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	478	GLU	CG-CD-OE2	-6.54	105.22	118.30
1	B	379	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	218	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
1	C	473	PHE	CB-CG-CD1	6.48	125.34	120.80
1	A	478	GLU	CG-CD-OE2	-6.39	105.53	118.30
1	B	192	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	D	103	PHE	CB-CG-CD2	6.35	125.24	120.80
1	B	478	GLU	CG-CD-OE1	6.34	130.99	118.30
1	C	76	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	554	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	510	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	192	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	205	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	454	PHE	CB-CG-CD2	-6.05	116.57	120.80
1	A	503	ASP	CB-CG-OD1	6.04	123.73	118.30
1	D	478	GLU	CG-CD-OE2	6.02	130.34	118.30
1	A	314	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	470	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	D	406	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	274	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	285	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	328	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	A	101	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	D	439	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	A	176	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	571	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	82	SER	CB-CA-C	-5.66	99.35	110.10
1	A	48	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	328	LEU	CB-CG-CD2	5.61	120.53	111.00
1	A	82	SER	CA-CB-OG	5.57	126.23	111.20
1	D	159	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	473	PHE	CB-CG-CD1	5.56	124.69	120.80
1	B	245	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	137	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	A	81	ASP	C-N-CA	5.50	135.46	121.70
1	A	472	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	C	349	LEU	CB-CG-CD2	5.45	120.27	111.00
1	B	201	LYS	CD-CE-NZ	-5.37	99.35	111.70
1	B	134	SER	N-CA-CB	5.30	118.45	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	CG-CD-NE	-5.28	100.72	111.80
1	A	383	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	328	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	D	211	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	D	554	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	138	VAL	CG1-CB-CG2	5.21	119.24	110.90
1	D	81	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	147	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	A	261	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	430	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	103	PHE	CB-CG-CD1	-5.14	117.20	120.80
1	B	60	THR	CA-CB-CG2	-5.12	105.23	112.40
1	B	288	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	349	LEU	CB-CG-CD2	5.04	119.57	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	THR	Peptide
1	B	436	THR	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	4571	0	4438	27	0
1	B	4595	0	4473	40	0
1	C	4531	0	4384	22	0
1	D	4561	0	4418	15	0
2	A	53	0	32	1	0
2	B	53	0	32	1	0
2	C	53	0	32	3	0
2	D	53	0	32	2	0
3	A	12	0	10	1	0
3	B	12	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	11	1	0
3	D	12	0	11	1	0
4	A	15	0	18	0	0
4	B	16	0	21	0	0
4	C	11	0	12	1	0
4	D	14	0	16	0	0
5	B	12	0	13	13	0
5	D	12	0	13	0	0
6	A	839	0	0	6	0
6	B	847	0	0	7	0
6	C	653	0	0	5	0
6	D	723	0	0	3	0
All	All	21660	0	17977	107	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 3.

All (107) 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:B:133:ALA:CB	5:B:804:MES:H71	1.44	1.43
1:B:133:ALA:HB3	5:B:804:MES:C7	1.59	1.32
1:A:393:VAL:N	1:A:417[B]:MET:HE3	1.51	1.23
1:B:133:ALA:CB	5:B:804:MES:C7	2.24	1.07
1:B:126:LEU:HD12	1:B:132[A]:GLN:CG	1.87	1.05
1:B:126:LEU:HD12	1:B:132[A]:GLN:HG3	1.43	0.98
1:A:393:VAL:H	1:A:417[B]:MET:HE3	1.31	0.95
1:A:393:VAL:HG23	1:A:417[B]:MET:CE	1.96	0.94
1:A:393:VAL:HG23	1:A:417[B]:MET:HE2	1.51	0.89
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.24	0.85
1:B:126:LEU:CD1	1:B:132[A]:GLN:CG	2.55	0.84
1:B:133:ALA:HB2	5:B:804:MES:H71	1.58	0.81
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.26	0.81
1:B:133:ALA:HB2	5:B:804:MES:O1S	1.81	0.80
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.27	0.80
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.34	0.76
1:A:462[B]:SER:OG	5:B:804:MES:H61	1.88	0.73
1:B:133:ALA:HB3	5:B:804:MES:H71	0.77	0.73
1:B:126:LEU:CD1	1:B:132[A]:GLN:HG2	2.17	0.72
4:C:803:12P:C5	6:C:1322:HOH:O	2.37	0.71
1:C:101:ASP:HB2	6:C:1375:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:VAL:N	1:A:417[B]:MET:CE	2.44	0.69
2:D:801:FDA:N5	3:D:802:2H5:H1	2.08	0.68
1:B:133:ALA:HB2	5:B:804:MES:C8	2.27	0.65
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.78	0.65
1:B:126:LEU:HD12	1:B:132[A]:GLN:HG2	1.70	0.64
1:A:82:SER:HB2	6:A:1064:HOH:O	1.97	0.64
1:B:133:ALA:HB2	5:B:804:MES:S	2.37	0.64
1:B:133:ALA:HB2	5:B:804:MES:C7	2.21	0.64
1:A:396[A]:THR:HG23	6:A:1717:HOH:O	1.99	0.63
1:A:102:LYS:NZ	6:A:1563:HOH:O	2.30	0.63
1:C:285:ARG:HD2	6:C:1433:HOH:O	1.97	0.62
1:A:50[A]:VAL:HG13	1:A:313:ALA:HB2	1.81	0.61
1:B:460:GLN:NE2	6:B:1617:HOH:O	2.33	0.60
2:C:801:FDA:N5	3:C:802:2H5:H1	2.17	0.60
1:A:393:VAL:HG23	1:A:417[B]:MET:HE3	1.79	0.59
1:B:50[B]:VAL:HG23	1:B:313:ALA:HB2	1.84	0.59
2:B:801:FDA:N5	3:B:802:2H5:H1	2.18	0.58
1:B:126:LEU:HD12	1:B:132[C]:GLN:HG3	1.85	0.58
1:A:392:SER:C	1:A:417[B]:MET:HE3	2.22	0.58
1:B:81:ASP:C	1:B:81:ASP:OD1	2.37	0.58
1:B:108:GLN:NE2	6:B:1292:HOH:O	2.38	0.57
1:C:82:SER:HB2	6:C:1036:HOH:O	2.03	0.57
1:B:133:ALA:CB	5:B:804:MES:C8	2.83	0.56
1:D:81:ASP:OD1	1:D:81:ASP:C	2.41	0.56
1:A:393:VAL:H	1:A:417[B]:MET:CE	2.14	0.55
1:A:50[B]:VAL:HG22	1:A:73:ALA:HB3	1.87	0.55
1:C:299:HIS:CD2	1:C:310:GLU:HG3	2.42	0.55
1:D:388:GLU:CB	1:D:390:THR:HG22	2.36	0.55
1:B:299:HIS:CD2	1:B:310:GLU:HG3	2.42	0.55
1:B:43[B]:MET:HG3	1:B:278:PHE:CE1	2.42	0.54
1:D:388:GLU:HB3	1:D:390:THR:HG22	1.90	0.54
1:B:299:HIS:NE2	1:B:310:GLU:HG2	2.23	0.54
1:A:393:VAL:CG2	1:A:417[B]:MET:HE2	2.33	0.53
1:B:347:GLU:HG3	6:B:1386:HOH:O	2.07	0.52
1:A:288:ARG:NH1	6:A:1412:HOH:O	2.42	0.52
1:C:459:VAL:HG13	1:C:461:GLN:HE21	1.74	0.52
1:D:462[C]:SER:OG	6:D:1477:HOH:O	2.20	0.51
1:C:215:GLU:O	1:C:411:LYS:NZ	2.44	0.50
1:B:132[C]:GLN:HE21	5:B:804:MES:H31	1.76	0.50
1:B:108:GLN:HG2	6:B:1611:HOH:O	2.11	0.50
1:A:393:VAL:CA	1:A:417[B]:MET:HE3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:HG2	1:B:348:LEU:HG	1.94	0.49
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.95	0.49
1:C:299:HIS:NE2	1:C:310:GLU:HG2	2.27	0.49
1:A:459:VAL:HG13	1:A:461:GLN:HE21	1.78	0.49
1:C:299:HIS:NE2	1:C:310:GLU:CG	2.77	0.48
1:D:108:GLN:NE2	6:D:1052:HOH:O	2.37	0.47
1:A:393:VAL:CG2	1:A:417[B]:MET:CE	2.81	0.46
2:A:801:FDA:N5	3:A:802:2H5:H1	2.30	0.46
1:D:214:LYS:HG3	1:D:215:GLU:HG3	1.98	0.46
1:B:513:LYS:NZ	6:B:1442:HOH:O	2.48	0.46
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.98	0.46
1:A:393:VAL:CG2	1:A:417[B]:MET:HE3	2.46	0.46
1:C:404:HIS:HB3	1:C:405:PRO:HD2	1.98	0.46
1:B:176:ASP:OD2	1:B:178:GLU:OE2	2.34	0.46
1:C:459:VAL:HG13	1:C:461:GLN:NE2	2.32	0.45
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.16	0.45
1:B:299:HIS:NE2	1:B:310:GLU:CG	2.80	0.44
1:C:47:TYR:O	1:C:313:ALA:HA	2.17	0.44
1:C:91:LYS:HD2	1:C:100:ILE:HD11	2.00	0.44
1:C:218:ARG:HD2	6:C:932:HOH:O	2.18	0.44
1:A:178:GLU:CD	1:A:439:PHE:HE1	2.21	0.43
1:C:169:THR:H	2:C:801:FDA:HN5	1.66	0.43
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.18	0.43
1:A:393:VAL:CB	1:A:417[B]:MET:HE3	2.47	0.43
1:C:169:THR:HB	2:C:801:FDA:O4	2.18	0.43
1:B:91:LYS:HD2	1:B:100:ILE:HD11	1.99	0.43
1:D:132:GLN:HG2	6:D:1613:HOH:O	2.18	0.43
1:A:108:GLN:NE2	6:A:1372:HOH:O	2.35	0.43
1:D:459:VAL:HG13	1:D:461:GLN:HE21	1.84	0.43
1:B:133:ALA:HB3	5:B:804:MES:H72	1.81	0.43
1:D:346:PRO:HG2	1:D:350:PRO:HA	2.00	0.42
1:B:358:GLU:HG2	1:B:544:GLY:HA2	2.02	0.42
1:B:91:LYS:CE	6:B:1710:HOH:O	2.68	0.42
1:A:185:LYS:HG2	1:A:557:PHE:CE2	2.55	0.42
1:C:265:ARG:HA	1:C:266:PRO:C	2.41	0.42
1:D:388:GLU:HB2	1:D:390:THR:HG22	2.01	0.41
1:B:607:GLU:HG3	6:B:1254:HOH:O	2.20	0.41
1:C:548:HIS:CD2	1:C:594:PRO:HD2	2.55	0.41
1:C:346:PRO:HG2	1:C:350:PRO:HA	2.02	0.41
1:A:481[B]:GLU:OE2	1:A:484:LYS:NZ	2.47	0.41
1:B:47:TYR:O	1:B:313:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:TYR:CE2	1:C:73:ALA:HB2	2.55	0.41
1:D:169:THR:H	2:D:801:FDA:HN5	1.68	0.41
1:D:185:LYS:HG2	1:D:557:PHE:CZ	2.56	0.40
6:A:1377:HOH:O	1:B:461:GLN:HG3	2.20	0.40

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	582/633 (92%)	569 (98%)	13 (2%)	0	100	100
1	B	585/633 (92%)	573 (98%)	12 (2%)	0	100	100
1	C	575/633 (91%)	562 (98%)	13 (2%)	0	100	100
1	D	580/633 (92%)	566 (98%)	14 (2%)	0	100	100
All	All	2322/2532 (92%)	2270 (98%)	52 (2%)	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	511/547 (93%)	506 (99%)	5 (1%)	82	62
1	B	515/547 (94%)	506 (98%)	9 (2%)	68	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	504/547 (92%)	495 (98%)	9 (2%)	66	35
1	D	509/547 (93%)	499 (98%)	10 (2%)	63	29
All	All	2039/2188 (93%)	2006 (98%)	33 (2%)	70	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	MET
1	A	168	TRP
1	A	206	PHE
1	A	408	TRP
1	A	593	ASN
1	B	112	MET
1	B	168	TRP
1	B	206	PHE
1	B	231	LYS
1	B	385[A]	THR
1	B	385[B]	THR
1	B	408	TRP
1	B	538	PRO
1	B	593	ASN
1	C	82	SER
1	C	112	MET
1	C	168	TRP
1	C	206	PHE
1	C	408	TRP
1	C	451	ARG
1	C	454	PHE
1	C	496	ASN
1	C	593	ASN
1	D	112	MET
1	D	168	TRP
1	D	206	PHE
1	D	383	ARG
1	D	385	THR
1	D	408	TRP
1	D	445	TRP
1	D	454	PHE
1	D	593	ASN
1	D	611	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	440	GLN
1	A	461	GLN
1	A	611	GLN
1	C	461	GLN
1	D	461	GLN
1	D	496	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](#)

14 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	1.56	8 (16%)	54,89,89	3.18	13 (24%)
3	2H5	A	802	-	12,12,12	2.32	3 (25%)	15,17,17	1.64	3 (20%)
4	12P	A	803	-	14,14,36	0.67	0	13,13,35	1.23	3 (23%)
2	FDA	B	801	1	48,58,58	1.29	7 (14%)	54,89,89	3.11	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2H5	B	802	-	12,12,12	1.27	2 (16%)	15,17,17	1.28	2 (13%)
4	12P	B	803	-	15,15,36	0.66	0	14,14,35	0.73	0
5	MES	B	804	-	11,12,12	1.39	1 (9%)	14,16,16	3.89	6 (42%)
2	FDA	C	801	1	48,58,58	1.63	11 (22%)	54,89,89	3.31	18 (33%)
3	2H5	C	802	-	12,12,12	1.58	2 (16%)	15,17,17	1.63	2 (13%)
4	12P	C	803	-	10,10,36	1.48	3 (30%)	9,9,35	2.54	3 (33%)
2	FDA	D	801	1	48,58,58	1.45	8 (16%)	54,89,89	2.52	18 (33%)
3	2H5	D	802	-	12,12,12	1.15	1 (8%)	15,17,17	2.20	3 (20%)
4	12P	D	803	-	13,13,36	0.66	0	12,12,35	0.78	0
5	MES	D	804	-	11,12,12	1.34	1 (9%)	14,16,16	2.09	1 (7%)

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	2H5	A	802	-	-	0/2/22/22	0/1/1/1
4	12P	A	803	-	-	0/12/12/34	0/0/0/0
2	FDA	B	801	1	-	0/30/50/50	0/6/6/6
3	2H5	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
2	FDA	C	801	1	-	0/30/50/50	0/6/6/6
3	2H5	C	802	-	-	0/2/22/22	0/1/1/1
4	12P	C	803	-	-	0/8/8/34	0/0/0/0
2	FDA	D	801	1	-	0/30/50/50	0/6/6/6
3	2H5	D	802	-	-	0/2/22/22	0/1/1/1
4	12P	D	803	-	-	0/11/11/34	0/0/0/0
5	MES	D	804	-	-	0/6/14/14	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	2H5	C3-C2	-5.08	1.47	1.52
3	A	802	2H5	C3-C4	-4.32	1.48	1.52
2	B	801	FDA	C2B-C3B	-4.08	1.42	1.53
2	D	801	FDA	O4B-C4B	-3.34	1.37	1.45
2	A	801	FDA	C9A-C5X	-2.91	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FDA	C4X-C10	-2.69	1.36	1.41
2	D	801	FDA	C9A-C5X	-2.57	1.37	1.42
2	B	801	FDA	C5A-C4A	-2.54	1.34	1.40
2	B	801	FDA	C9A-C5X	-2.32	1.37	1.42
2	A	801	FDA	C1'-N10	-2.26	1.46	1.48
3	B	802	2H5	C3-C4	-2.21	1.50	1.52
2	C	801	FDA	C10-N10	-2.20	1.36	1.39
3	C	802	2H5	C1-C2	-2.13	1.48	1.52
2	C	801	FDA	C4X-C10	-2.12	1.37	1.41
2	C	801	FDA	C8A-N7A	-2.04	1.30	1.34
2	C	801	FDA	O2B-C2B	-2.03	1.38	1.43
2	D	801	FDA	C4'-C3'	2.06	1.57	1.53
2	B	801	FDA	C9-C9A	2.09	1.45	1.40
2	C	801	FDA	C6-C5X	2.10	1.44	1.41
4	C	803	12P	O7-C8	2.12	1.51	1.42
2	B	801	FDA	C7M-C7	2.15	1.55	1.51
5	D	804	MES	C5-N4	2.19	1.52	1.46
2	A	801	FDA	C4X-N5	2.22	1.36	1.33
2	B	801	FDA	C2A-N3A	2.23	1.36	1.32
2	C	801	FDA	C4-C4X	2.25	1.45	1.41
2	C	801	FDA	C2A-N3A	2.38	1.36	1.32
2	C	801	FDA	C9-C8	2.44	1.44	1.37
2	A	801	FDA	C5A-C4A	2.46	1.46	1.40
4	C	803	12P	O10-C9	2.48	1.52	1.42
2	D	801	FDA	C10-N1	2.53	1.39	1.35
2	A	801	FDA	C2'-C3'	2.58	1.58	1.53
2	D	801	FDA	C4-C4X	2.59	1.46	1.41
4	C	803	12P	C8-C9	2.63	1.62	1.48
2	D	801	FDA	C9A-N10	2.65	1.42	1.38
5	B	804	MES	O2S-S	2.67	1.53	1.45
2	B	801	FDA	O4B-C1B	2.73	1.44	1.41
3	B	802	2H5	C4-C5	2.80	1.59	1.53
2	D	801	FDA	C7M-C7	2.87	1.56	1.51
2	A	801	FDA	C2A-N3A	2.90	1.37	1.32
3	D	802	2H5	C4-C5	2.98	1.59	1.53
2	C	801	FDA	C7M-C7	3.25	1.57	1.51
3	A	802	2H5	C4-C5	3.58	1.60	1.53
3	C	802	2H5	C3-C4	3.61	1.55	1.52
2	D	801	FDA	C4-N3	3.79	1.40	1.33
2	C	801	FDA	C4-N3	4.11	1.40	1.33
2	A	801	FDA	C4-C4X	4.71	1.50	1.41
2	C	801	FDA	C4X-N5	5.44	1.41	1.33

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FDA	C4X-C4-N3	-10.38	109.39	123.59
2	B	801	FDA	C4-C4X-C10	-10.02	113.53	119.94
2	B	801	FDA	N3A-C2A-N1A	-9.25	121.81	128.89
5	B	804	MES	O2S-S-C8	-9.09	99.15	106.91
2	A	801	FDA	N3A-C2A-N1A	-8.73	122.21	128.89
2	A	801	FDA	C4X-C4-N3	-7.95	112.72	123.59
2	C	801	FDA	N3A-C2A-N1A	-7.86	122.88	128.89
2	D	801	FDA	C4A-C5A-N7A	-7.18	102.87	109.48
3	D	802	2H5	F3-C3-C4	-5.57	104.57	108.52
2	A	801	FDA	C4X-C10-N10	-5.14	117.49	120.52
2	D	801	FDA	C4X-C4-N3	-4.86	116.95	123.59
2	B	801	FDA	C6-C5X-N5	-4.75	112.84	118.96
2	C	801	FDA	C4-C4X-N5	-4.69	113.03	118.72
3	C	802	2H5	F3-C3-C2	-4.47	105.35	108.52
2	A	801	FDA	C4A-C5A-N7A	-4.35	105.48	109.48
3	A	802	2H5	F3-C3-C2	-4.10	105.61	108.52
5	B	804	MES	O3S-S-O2S	-4.03	102.23	111.61
2	B	801	FDA	C4X-C4-N3	-3.98	118.14	123.59
2	B	801	FDA	C4A-C5A-N7A	-3.78	106.00	109.48
2	B	801	FDA	C4X-C10-N10	-3.56	118.42	120.52
2	D	801	FDA	C4X-N5-C5X	-3.54	112.69	116.76
2	C	801	FDA	C6-C5X-N5	-3.44	114.54	118.96
5	B	804	MES	O1-C6-C5	-3.40	104.05	111.84
2	C	801	FDA	C4X-N5-C5X	-2.73	113.63	116.76
2	D	801	FDA	C6-C5X-C9A	-2.72	115.41	118.98
2	B	801	FDA	C9-C9A-C5X	-2.57	115.04	119.62
2	D	801	FDA	C9-C8-C7	-2.54	115.18	120.04
4	A	803	12P	C9-O10-C11	-2.53	102.43	113.31
5	B	804	MES	O1-C2-C3	-2.50	106.10	111.84
2	A	801	FDA	C9A-C5X-N5	-2.49	118.68	122.36
2	A	801	FDA	C4-C4X-C10	-2.28	118.48	119.94
3	A	802	2H5	O5-C5-C4	-2.28	105.40	109.68
2	C	801	FDA	C1B-N9A-C4A	-2.25	123.55	126.94
2	C	801	FDA	C5X-C9A-N10	-2.17	115.97	117.62
3	C	802	2H5	C3-C2-C1	-2.14	106.39	110.46
2	A	801	FDA	C6-C7-C8	-2.12	116.00	120.04
2	D	801	FDA	N3A-C2A-N1A	-2.10	127.29	128.89
4	A	803	12P	O10-C11-C12	-2.09	101.08	110.36
3	B	802	2H5	O2-C2-C3	-2.07	105.35	109.05
2	C	801	FDA	O2B-C2B-C3B	2.01	118.37	111.83
2	C	801	FDA	O2A-PA-O1A	2.02	123.45	112.53
2	C	801	FDA	N6A-C6A-N1A	2.05	123.61	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	12P	C3-O4-C5	2.08	120.76	112.80
2	D	801	FDA	O3'-C3'-C2'	2.10	114.05	108.75
5	B	804	MES	C5-N4-C3	2.11	113.46	108.90
4	C	803	12P	C14-O13-C12	2.11	120.89	112.80
2	C	801	FDA	C9A-C5X-N5	2.18	125.58	122.36
2	D	801	FDA	O2A-PA-O1A	2.26	124.77	112.53
3	A	802	2H5	O4-C4-C3	2.35	113.25	109.05
2	D	801	FDA	O3B-C3B-C4B	2.39	118.22	111.05
2	A	801	FDA	C2A-N1A-C6A	2.42	123.10	118.77
2	D	801	FDA	C2A-N1A-C6A	2.49	123.22	118.77
2	D	801	FDA	O2B-C2B-C3B	2.52	120.02	111.83
2	D	801	FDA	O2'-C2'-C3'	2.54	115.40	109.02
2	B	801	FDA	C2B-C3B-C4B	2.54	107.84	102.61
2	B	801	FDA	O2B-C2B-C3B	2.54	120.09	111.83
2	C	801	FDA	C8M-C8-C7	2.56	126.34	120.73
2	D	801	FDA	C1B-N9A-C4A	2.59	130.85	126.94
2	B	801	FDA	C8M-C8-C7	2.66	126.57	120.73
2	B	801	FDA	C2A-N1A-C6A	2.78	123.73	118.77
2	C	801	FDA	C2B-C1B-N9A	2.80	118.57	114.29
3	B	802	2H5	O4-C4-C3	2.87	114.18	109.05
2	C	801	FDA	C1'-N10-C9A	2.94	122.16	118.86
2	D	801	FDA	C4X-C10-N10	3.38	122.51	120.52
3	D	802	2H5	O2-C2-C1	3.48	117.48	109.82
2	B	801	FDA	C6-C5X-C9A	3.56	123.66	118.98
2	D	801	FDA	C9A-C5X-N5	3.81	128.00	122.36
2	B	801	FDA	C1'-N10-C9A	3.82	123.15	118.86
4	C	803	12P	C9-O10-C11	3.83	129.77	113.31
2	A	801	FDA	C1B-N9A-C4A	3.94	132.89	126.94
2	B	801	FDA	C4-C4X-N5	3.99	123.56	118.72
2	A	801	FDA	C2B-C3B-C4B	4.03	110.89	102.61
2	C	801	FDA	C2A-N1A-C6A	4.07	126.04	118.77
2	A	801	FDA	C5X-C9A-N10	4.26	120.86	117.62
3	D	802	2H5	O5-C1-C2	4.34	116.73	109.80
2	D	801	FDA	C2B-C1B-N9A	4.45	121.09	114.29
4	C	803	12P	O7-C8-C9	5.83	136.29	110.36
2	D	801	FDA	C4-N3-C2	6.81	121.13	115.25
5	D	804	MES	O2S-S-C8	7.02	112.89	106.91
2	C	801	FDA	C4X-C10-N10	7.03	124.66	120.52
2	A	801	FDA	C1'-N10-C9A	7.37	127.14	118.86
2	D	801	FDA	C1'-N10-C9A	7.79	127.61	118.86
5	B	804	MES	O1S-S-C8	9.18	114.74	106.91
2	C	801	FDA	C4-N3-C2	10.08	123.96	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FDA	C4-C4X-C10	10.91	126.92	119.94
2	B	801	FDA	C4-N3-C2	12.00	125.62	115.25
2	A	801	FDA	C4-N3-C2	13.49	126.91	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
2	A	801	FDA	1	0
3	A	802	2H5	1	0
2	B	801	FDA	1	0
3	B	802	2H5	1	0
5	B	804	MES	13	0
2	C	801	FDA	3	0
3	C	802	2H5	1	0
4	C	803	12P	1	0
2	D	801	FDA	2	0
3	D	802	2H5	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, 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%)	-0.35	13 (2%) 64 67	13, 19, 35, 61	0
1	B	576/633 (90%)	-0.30	10 (1%) 73 76	13, 18, 34, 63	0
1	C	573/633 (90%)	-0.18	15 (2%) 59 63	16, 27, 47, 75	0
1	D	576/633 (90%)	-0.24	10 (1%) 73 76	15, 23, 43, 94	0
All	All	2301/2532 (90%)	-0.27	48 (2%) 67 70	13, 22, 41, 94	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	618	PHE	9.5
1	D	389	LEU	5.3
1	B	618	PHE	4.8
1	C	343	ALA	4.7
1	D	345	PRO	4.4
1	D	385	THR	4.3
1	C	270	ALA	4.1
1	B	343	ALA	4.1
1	B	345	PRO	4.0
1	A	618	PHE	4.0
1	D	618	PHE	3.9
1	D	390	THR	3.9
1	B	45	ILE	3.8
1	C	345	PRO	3.6
1	D	343	ALA	3.5
1	B	389	LEU	3.5
1	C	344	ASN	3.5
1	D	382	ILE	3.5
1	C	271	PRO	3.5
1	A	343	ALA	3.4
1	C	269	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	272	GLU	3.3
1	C	617	PRO	3.2
1	A	385	THR	3.2
1	A	387	GLY	3.1
1	A	389	LEU	3.1
1	D	383	ARG	3.0
1	D	388	GLU	3.0
1	B	268	THR	2.9
1	B	344	ASN	2.8
1	A	401	THR	2.8
1	A	268	THR	2.6
1	C	268	THR	2.6
1	A	344	ASN	2.5
1	D	44	ASP	2.5
1	B	132[A]	GLN	2.5
1	A	388	GLU	2.5
1	C	616	SER	2.5
1	A	384	GLY	2.5
1	B	342	PRO	2.4
1	C	385	THR	2.4
1	C	266	PRO	2.4
1	A	345	PRO	2.4
1	A	400	SER	2.2
1	A	82	SER	2.2
1	C	310	GLU	2.1
1	B	400	SER	2.1
1	C	388	GLU	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 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
4	12P	A	803	15/37	0.87	0.10	6.71	25,32,43,48	0
4	12P	C	803	11/37	0.80	0.12	2.56	27,31,34,35	0
4	12P	D	803	14/37	0.92	0.09	1.89	24,30,40,42	0
4	12P	B	803	16/37	0.94	0.07	1.25	26,28,48,61	0
5	MES	B	804	12/12	0.94	0.22	1.20	22,30,33,35	0
5	MES	D	804	12/12	0.96	0.11	0.53	28,31,40,42	0
3	2H5	C	802	12/12	0.95	0.07	0.02	22,23,24,24	0
3	2H5	B	802	12/12	0.97	0.07	-0.36	15,17,19,19	0
2	FDA	C	801	53/53	0.96	0.06	-0.37	18,22,24,27	0
3	2H5	D	802	12/12	0.97	0.06	-0.85	19,20,23,23	0
2	FDA	A	801	53/53	0.98	0.06	-0.87	12,14,16,17	0
2	FDA	D	801	53/53	0.97	0.06	-0.93	14,17,22,23	0
2	FDA	B	801	53/53	0.98	0.06	-1.06	11,13,15,17	0
3	2H5	A	802	12/12	0.97	0.06	-1.83	16,18,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.