wwPDB X-ray Structure Validation Summary Report (i)

Feb 9, 2021 – 04:11 PM GMT

PDB ID	:	7AM6
Title	:	Crystal structure of Peptiligase mutant - L217H/M222P/A225N/F189W
Authors	:	Rozeboom, H.J.; Janssen, D.J.
Deposited on	:	2020-10-08
Resolution	:	2.70 Å(reported)

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

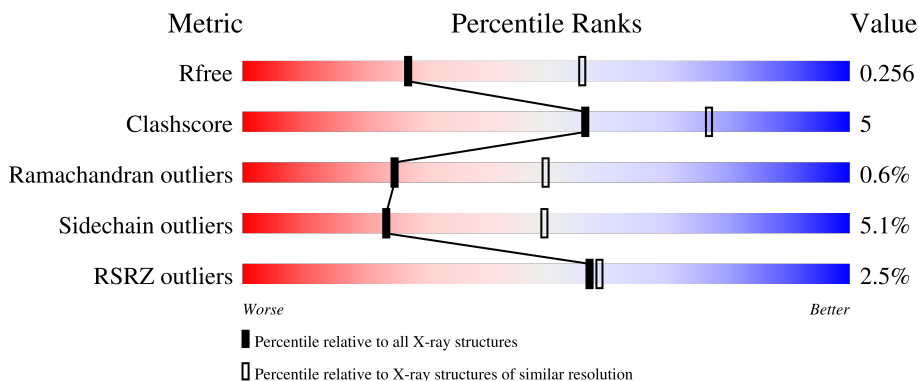|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.70 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		0.256
Clashscore		5
Ramachandran outliers		0.6%
Sidechain outliers		5.1%
RSRZ outliers		2.5%

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	272	3% / 84% / 14% ·
1	C	272	3% / 86% / 12% ··
2	B	272	86% / 13% ·
3	P	13	15% / 15% / 23% / 15% / 46%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5841 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 Subtilisin BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total 1886	C 1172	N 328	O 380	S 6	0	0	0
1	C	267	Total 1890	C 1173	N 332	O 379	S 6	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	GLN	engineered mutation	UNP P00782
A	3	CYS	SER	engineered mutation	UNP P00782
A	5	SER	PRO	engineered mutation	UNP P00782
A	43	ASN	LYS	engineered mutation	UNP P00782
A	50	PHE	MET	engineered mutation	UNP P00782
A	?	-	ALA	deletion	UNP P00782
A	?	-	ALA	deletion	UNP P00782
A	?	-	LEU	deletion	UNP P00782
A	?	-	ASN	deletion	UNP P00782
A	?	-	ASN	deletion	UNP P00782
A	?	-	SER	deletion	UNP P00782
A	?	-	ILE	deletion	UNP P00782
A	?	-	GLY	deletion	UNP P00782
A	?	-	VAL	deletion	UNP P00782
A	74	ALA	GLY	engineered mutation	UNP P00782
A	156	SER	GLU	engineered mutation	UNP P00782
A	166	SER	GLY	engineered mutation	UNP P00782
A	169	ALA	GLY	engineered mutation	UNP P00782
A	188	PRO	SER	engineered mutation	UNP P00782
A	189	TRP	PHE	engineered mutation	UNP P00782
A	206	CYS	GLN	engineered mutation	UNP P00782
A	217	HIS	TYR	engineered mutation	UNP P00782
A	218	SER	ASN	engineered mutation	UNP P00782
A	221	CSO	SER	engineered mutation	UNP P00782
A	222	PRO	MET	engineered mutation	UNP P00782

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Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ASN	PRO	engineered mutation	UNP P00782
A	254	ALA	THR	engineered mutation	UNP P00782
A	271	GLU	GLN	engineered mutation	UNP P00782
A	276	HIS	-	expression tag	UNP P00782
A	277	HIS	-	expression tag	UNP P00782
A	278	HIS	-	expression tag	UNP P00782
A	279	HIS	-	expression tag	UNP P00782
A	280	HIS	-	expression tag	UNP P00782
A	281	HIS	-	expression tag	UNP P00782
C	2	LYS	GLN	engineered mutation	UNP P00782
C	3	CYS	SER	engineered mutation	UNP P00782
C	5	SER	PRO	engineered mutation	UNP P00782
C	43	ASN	LYS	engineered mutation	UNP P00782
C	50	PHE	MET	engineered mutation	UNP P00782
C	?	-	ALA	deletion	UNP P00782
C	?	-	ALA	deletion	UNP P00782
C	?	-	LEU	deletion	UNP P00782
C	?	-	ASN	deletion	UNP P00782
C	?	-	ASN	deletion	UNP P00782
C	?	-	SER	deletion	UNP P00782
C	?	-	ILE	deletion	UNP P00782
C	?	-	GLY	deletion	UNP P00782
C	?	-	VAL	deletion	UNP P00782
C	74	ALA	GLY	engineered mutation	UNP P00782
C	156	SER	GLU	engineered mutation	UNP P00782
C	166	SER	GLY	engineered mutation	UNP P00782
C	169	ALA	GLY	engineered mutation	UNP P00782
C	188	PRO	SER	engineered mutation	UNP P00782
C	189	TRP	PHE	engineered mutation	UNP P00782
C	206	CYS	GLN	engineered mutation	UNP P00782
C	217	HIS	TYR	engineered mutation	UNP P00782
C	218	SER	ASN	engineered mutation	UNP P00782
C	221	CSO	SER	engineered mutation	UNP P00782
C	222	PRO	MET	engineered mutation	UNP P00782
C	225	ASN	PRO	engineered mutation	UNP P00782
C	254	ALA	THR	engineered mutation	UNP P00782
C	271	GLU	GLN	engineered mutation	UNP P00782
C	276	HIS	-	expression tag	UNP P00782
C	277	HIS	-	expression tag	UNP P00782
C	278	HIS	-	expression tag	UNP P00782
C	279	HIS	-	expression tag	UNP P00782
C	280	HIS	-	expression tag	UNP P00782

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Chain	Residue	Modelled	Actual	Comment	Reference
C	281	HIS	-	expression tag	UNP P00782

- Molecule 2 is a protein called Subtilisin BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	269	1905	1184	334	381	6	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	LYS	GLN	engineered mutation	UNP P00782
B	3	CYS	SER	engineered mutation	UNP P00782
B	5	SER	PRO	engineered mutation	UNP P00782
B	43	ASN	LYS	engineered mutation	UNP P00782
B	50	PHE	MET	engineered mutation	UNP P00782
B	?	-	ALA	engineered mutation	UNP P00782
B	?	-	ALA	deletion	UNP P00782
B	?	-	LEU	deletion	UNP P00782
B	?	-	ASN	deletion	UNP P00782
B	?	-	ASN	deletion	UNP P00782
B	?	-	SER	deletion	UNP P00782
B	?	-	ILE	deletion	UNP P00782
B	?	-	GLY	deletion	UNP P00782
B	?	-	VAL	deletion	UNP P00782
B	74	ALA	GLY	engineered mutation	UNP P00782
B	156	SER	GLU	engineered mutation	UNP P00782
B	166	SER	GLY	engineered mutation	UNP P00782
B	169	ALA	GLY	engineered mutation	UNP P00782
B	188	PRO	SER	engineered mutation	UNP P00782
B	189	TRP	PHE	engineered mutation	UNP P00782
B	206	CYS	GLN	engineered mutation	UNP P00782
B	217	HIS	TYR	engineered mutation	UNP P00782
B	218	SER	ASN	engineered mutation	UNP P00782
B	221	CYS	SER	engineered mutation	UNP P00782
B	222	PRO	MET	engineered mutation	UNP P00782
B	225	ASN	PRO	engineered mutation	UNP P00782
B	254	ALA	THR	engineered mutation	UNP P00782
B	271	GLU	GLN	engineered mutation	UNP P00782
B	276	HIS	-	expression tag	UNP P00782
B	277	HIS	-	expression tag	UNP P00782
B	278	HIS	-	expression tag	UNP P00782

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Chain	Residue	Modelled	Actual	Comment	Reference
B	279	HIS	-	expression tag	UNP P00782
B	280	HIS	-	expression tag	UNP P00782
B	281	HIS	-	expression tag	UNP P00782

- Molecule 3 is a protein called LEU-PRO-GLU-GLY-SER-PRO-VAL-THR-ASP-LEU-ARG-TYR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	7	47	29	7	11	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
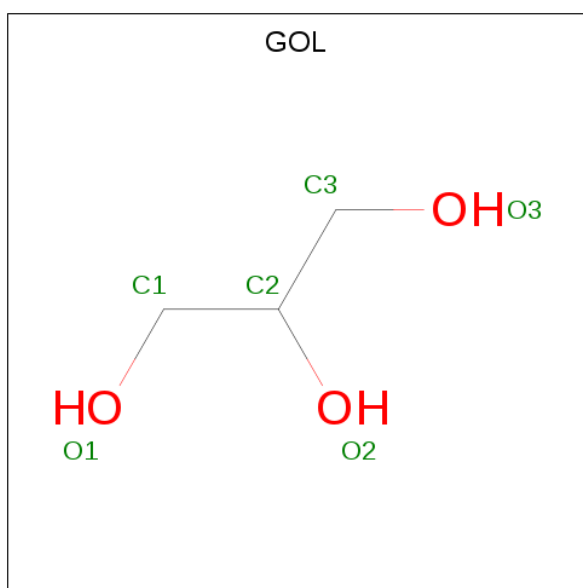
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).

TAR
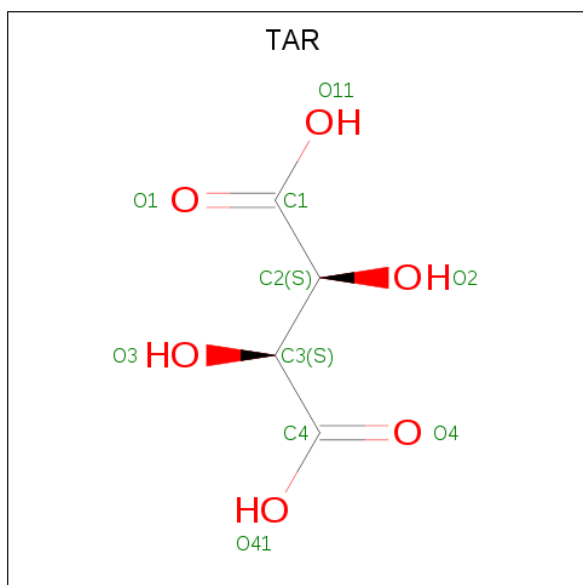
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	4	6		
5	C	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total	O	0	0
			15	15		
6	B	21	Total	O	0	0
			21	21		
6	C	9	Total	O	0	0
			9	9		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
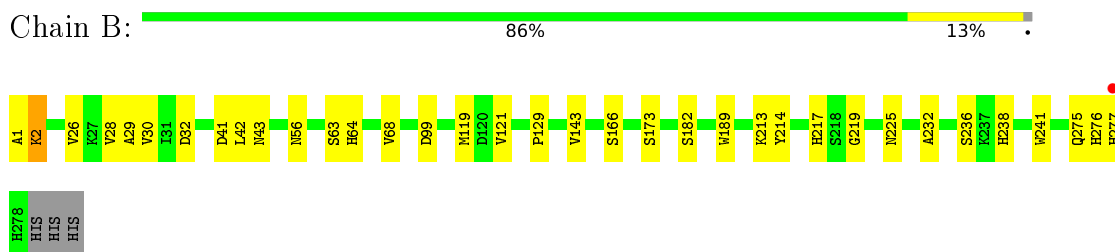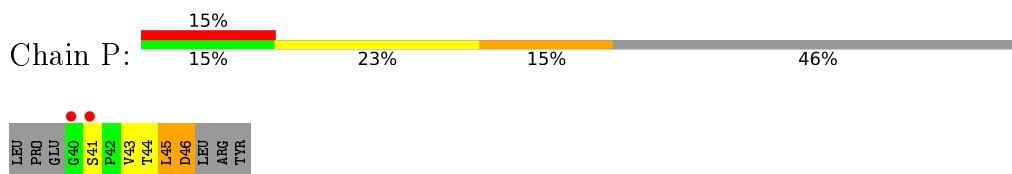
- Molecule 1: Subtilisin BPN'
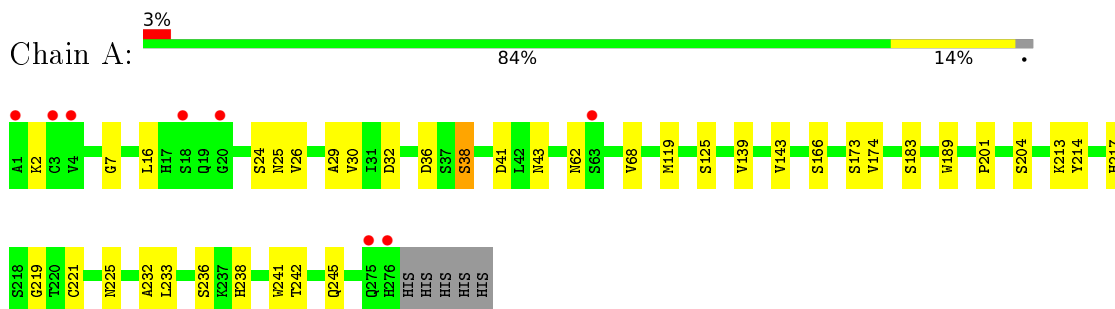
- Molecule 1: Subtilisin BPN'
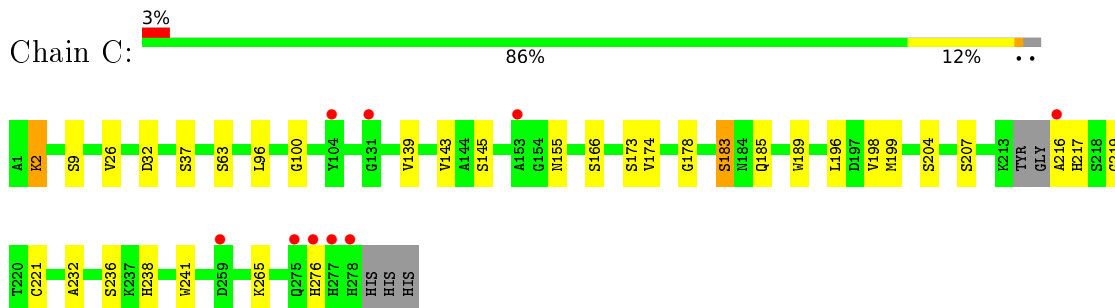
- Molecule 2: Subtilisin BPN'

- Molecule 3: LEU-PRO-GLU-GLY-SER-PRO-VAL-THR-ASP-LEU-ARG-TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	105.44Å 105.44Å 192.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.70 58.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (58.96-2.70) 96.2 (58.89-2.70)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.59 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.212 , 0.252 0.217 , 0.256	Depositor DCC
R_{free} test set	1458 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.6	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5841	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: GOL, CSO, TAR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.76	0/1919	0.88	0/2622
1	C	0.78	0/1923	0.90	0/2626
2	B	0.80	0/1948	0.91	0/2664
3	P	0.95	0/47	1.26	0/64
All	All	0.78	0/5837	0.90	0/7976

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
3	P	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	45	LEU	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	1886	0	1834	16	0
1	C	1890	0	1835	24	0
2	B	1905	0	1847	17	0
3	P	47	0	45	11	0
4	A	6	0	8	0	0
4	B	30	0	40	1	0
4	C	12	0	16	0	0
5	B	10	0	4	1	0
5	C	10	0	4	0	0
6	A	15	0	0	0	0
6	B	21	0	0	0	0
6	C	9	0	0	0	0
All	All	5841	0	5633	57	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 5.

The worst 5 of 57 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ASN:HD21	3:P:46:ASP:H	1.22	0.87
1:C:155:ASN:ND2	3:P:46:ASP:H	1.76	0.82
1:C:221:CSO:HB2	3:P:46:ASP:HB3	1.59	0.82
1:C:183:SER:OG	1:C:185:GLN:HG2	1.94	0.68
1:C:196:LEU:HD11	1:C:199:MET:HE1	1.80	0.63

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	264/272 (97%)	255 (97%)	8 (3%)	1 (0%)	34 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	262/272 (96%)	254 (97%)	6 (2%)	2 (1%)	19	43
2	B	267/272 (98%)	260 (97%)	5 (2%)	2 (1%)	22	46
3	P	5/13 (38%)	4 (80%)	1 (20%)	0	100	100
All	All	798/829 (96%)	773 (97%)	20 (2%)	5 (1%)	25	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
2	B	2	LYS
1	C	276	HIS
2	B	276	HIS
1	C	63	SER

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	199/204 (98%)	189 (95%)	10 (5%)	24	51
1	C	200/204 (98%)	189 (94%)	11 (6%)	21	46
2	B	202/205 (98%)	194 (96%)	8 (4%)	31	60
3	P	6/12 (50%)	4 (67%)	2 (33%)	0	0
All	All	607/625 (97%)	576 (95%)	31 (5%)	24	50

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	182	SER
2	B	236	SER
1	C	265	LYS
2	B	213	LYS
1	C	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	43	ASN
2	B	123	ASN
1	C	61	ASN
2	B	19	GLN
2	B	277	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	CSO	C	221	1	3,6,7	1.00	0	0,6,8	0.00	-
1	CSO	A	221	1	3,6,7	1.01	0	0,6,8	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	C	221	1	-	1/1/5/7	-
1	CSO	A	221	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	221	CSO	N-CA-CB-SG
1	A	221	CSO	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	221	CSO	2	0
1	A	221	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	GOL	B	303	-	5,5,5	0.12	0	5,5,5	0.31	0
5	TAR	C	301	-	3,9,9	0.62	0	6,12,12	1.67	1 (16%)
4	GOL	C	303	-	5,5,5	0.09	0	5,5,5	0.27	0
5	TAR	B	301	2	3,9,9	1.31	0	6,12,12	2.24	4 (66%)
4	GOL	B	306	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	B	302	-	5,5,5	0.13	0	5,5,5	0.31	0
4	GOL	B	305	-	5,5,5	0.16	0	5,5,5	0.38	0
4	GOL	A	301	-	5,5,5	0.14	0	5,5,5	0.31	0
4	GOL	C	302	-	5,5,5	0.09	0	5,5,5	0.29	0
4	GOL	B	304	-	5,5,5	0.15	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	303	-	-	2/4/4/4	-
5	TAR	C	301	-	-	4/4/12/12	-
4	GOL	C	303	-	-	2/4/4/4	-
5	TAR	B	301	2	-	4/4/12/12	-
4	GOL	B	306	-	-	0/4/4/4	-
4	GOL	B	302	-	-	3/4/4/4	-
4	GOL	B	305	-	-	2/4/4/4	-
4	GOL	A	301	-	-	0/4/4/4	-
4	GOL	C	302	-	-	1/4/4/4	-
4	GOL	B	304	-	-	2/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301	TAR	O3-C3-C4	-3.67	102.26	111.10
5	C	301	TAR	C4-C3-C2	-3.20	106.23	113.11
5	B	301	TAR	O3-C3-C2	2.50	117.25	108.90
5	B	301	TAR	C4-C3-C2	2.08	117.57	113.11
5	B	301	TAR	C1-C2-C3	2.07	117.56	113.11

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	301	TAR	C1-C2-C3-O3
5	C	301	TAR	O2-C2-C3-O3
5	C	301	TAR	O2-C2-C3-C4
4	C	303	GOL	C1-C2-C3-O3
5	B	301	TAR	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	GOL	1	0
5	B	301	TAR	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	266/272 (97%)	0.06	8 (3%)	50	51	22, 36, 59, 113	0
1	C	266/272 (97%)	0.29	9 (3%)	45	45	27, 43, 64, 108	0
2	B	269/272 (98%)	-0.09	1 (0%)	92	93	22, 32, 47, 105	0
3	P	7/13 (53%)	1.73	2 (28%)	0	0	68, 78, 90, 99	0
All	All	808/829 (97%)	0.10	20 (2%)	57	59	22, 36, 62, 113	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	277	HIS	5.3
1	C	278	HIS	4.2
1	A	1	ALA	3.9
1	A	276	HIS	3.7
1	A	4	VAL	3.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
1	CSO	C	221	7/8	0.90	0.17	45,48,53,57	0
1	CSO	A	221	7/8	0.93	0.12	31,33,35,38	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
4	GOL	B	306	6/6	0.80	0.20	52,57,59,59	0
4	GOL	C	303	6/6	0.82	0.34	77,81,84,84	0
4	GOL	C	302	6/6	0.84	0.25	58,60,61,61	0
5	TAR	C	301	10/10	0.86	0.32	53,61,70,72	0
4	GOL	A	301	6/6	0.86	0.26	45,58,61,62	0
5	TAR	B	301	10/10	0.86	0.19	37,50,61,69	0
4	GOL	B	305	6/6	0.87	0.20	47,55,60,62	0
4	GOL	B	303	6/6	0.88	0.14	57,59,61,61	0
4	GOL	B	304	6/6	0.88	0.18	50,54,57,57	0
4	GOL	B	302	6/6	0.89	0.23	46,48,49,53	0

6.5 Other polymers (i)

There are no such residues in this entry.