wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 03:23 PM EDT

PDB ID	:	3GDV
Title	:	Crystal structure of DegS H198P/D320A mutant modified by DFP and in complex with YQF peptide
Authors	:	Sohn, J.; Grant, R.A.; Sauer, R.T.
Deposited on	:	2009-02-24
Resolution	:	2.49 Å(reported)

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

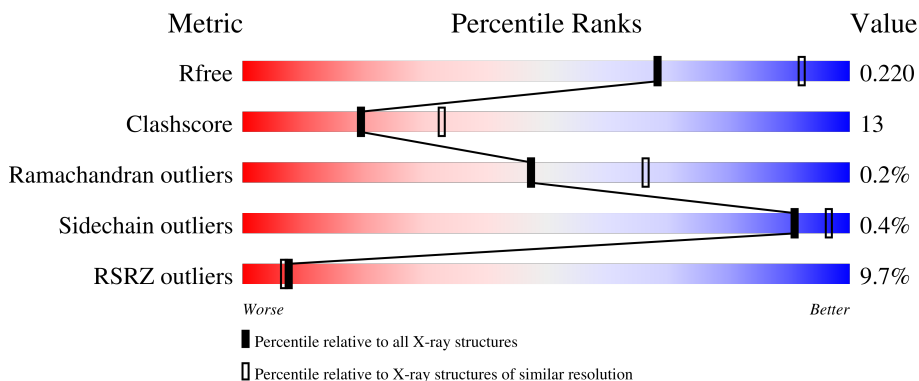|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.49 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		0.220
Clashscore		13
Ramachandran outliers		0.2%
Sidechain outliers		0.4%
RSRZ outliers		9.7%

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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	340	6% 65% 22% 13%
1	B	340	14% 66% 18% 16%
1	C	340	4% 69% 17% 14%
2	D	3	67% 67% 33%
2	E	3	100% 67% 33%

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Mol	Chain	Length	Quality of chain
2	F	3	33% 67%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6662 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 DegS protease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	0	0
			2193	1371	388	428	1	5			
1	B	284	Total	C	N	O	P	S	0	0	0
			2103	1321	367	410	1	4			
1	C	294	Total	C	N	O	P	S	0	0	0
			2189	1372	388	423	1	5			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP P0AEE3
A	17	ARG	-	expression tag	UNP P0AEE3
A	18	GLY	-	expression tag	UNP P0AEE3
A	19	SER	-	expression tag	UNP P0AEE3
A	20	HIS	-	expression tag	UNP P0AEE3
A	21	HIS	-	expression tag	UNP P0AEE3
A	22	HIS	-	expression tag	UNP P0AEE3
A	23	HIS	-	expression tag	UNP P0AEE3
A	24	HIS	-	expression tag	UNP P0AEE3
A	25	HIS	-	expression tag	UNP P0AEE3
A	26	GLY	-	expression tag	UNP P0AEE3
A	198	PRO	HIS	engineered mutation	UNP P0AEE3
A	320	ALA	ASP	engineered mutation	UNP P0AEE3
B	16	MET	-	expression tag	UNP P0AEE3
B	17	ARG	-	expression tag	UNP P0AEE3
B	18	GLY	-	expression tag	UNP P0AEE3
B	19	SER	-	expression tag	UNP P0AEE3
B	20	HIS	-	expression tag	UNP P0AEE3
B	21	HIS	-	expression tag	UNP P0AEE3
B	22	HIS	-	expression tag	UNP P0AEE3
B	23	HIS	-	expression tag	UNP P0AEE3
B	24	HIS	-	expression tag	UNP P0AEE3
B	25	HIS	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	expression tag	UNP P0AEE3
B	198	PRO	HIS	engineered mutation	UNP P0AEE3
B	320	ALA	ASP	engineered mutation	UNP P0AEE3
C	16	MET	-	expression tag	UNP P0AEE3
C	17	ARG	-	expression tag	UNP P0AEE3
C	18	GLY	-	expression tag	UNP P0AEE3
C	19	SER	-	expression tag	UNP P0AEE3
C	20	HIS	-	expression tag	UNP P0AEE3
C	21	HIS	-	expression tag	UNP P0AEE3
C	22	HIS	-	expression tag	UNP P0AEE3
C	23	HIS	-	expression tag	UNP P0AEE3
C	24	HIS	-	expression tag	UNP P0AEE3
C	25	HIS	-	expression tag	UNP P0AEE3
C	26	GLY	-	expression tag	UNP P0AEE3
C	198	PRO	HIS	engineered mutation	UNP P0AEE3
C	320	ALA	ASP	engineered mutation	UNP P0AEE3

- Molecule 2 is a protein called YQF peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total 33	C 23	N 4	O 6	0	0	0
2	E	3	Total 33	C 23	N 4	O 6	0	0	0
2	F	3	Total 33	C 23	N 4	O 6	0	0	0

- Molecule 3 is water.

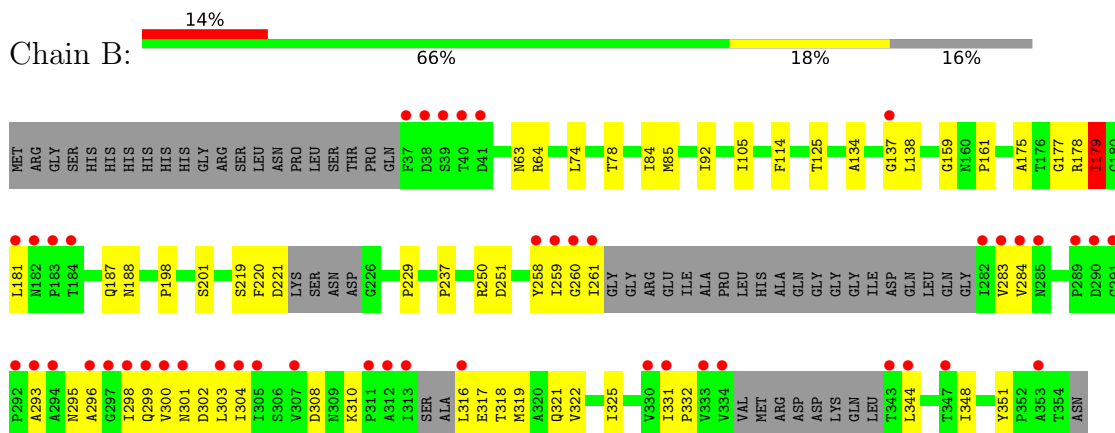| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	34	Total 34	O 34	0	0
3	C	32	Total 32	O 32	0	0

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.
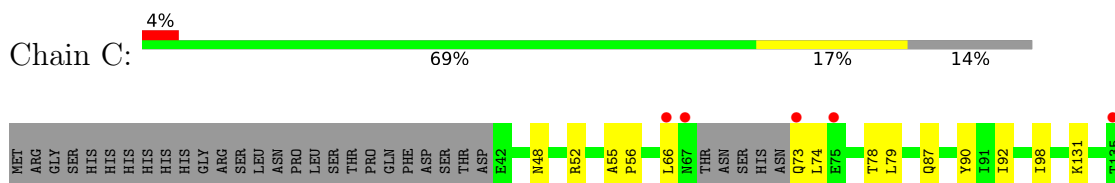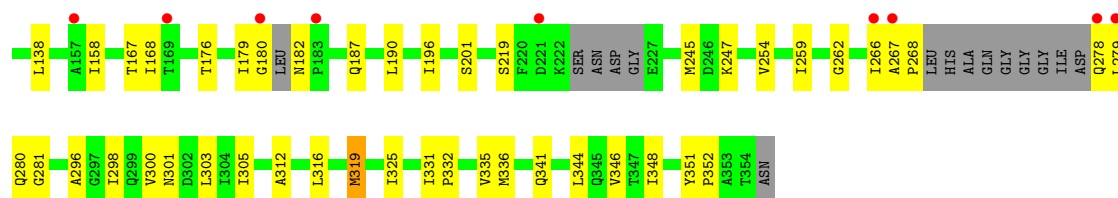
- Molecule 1: DegS protease
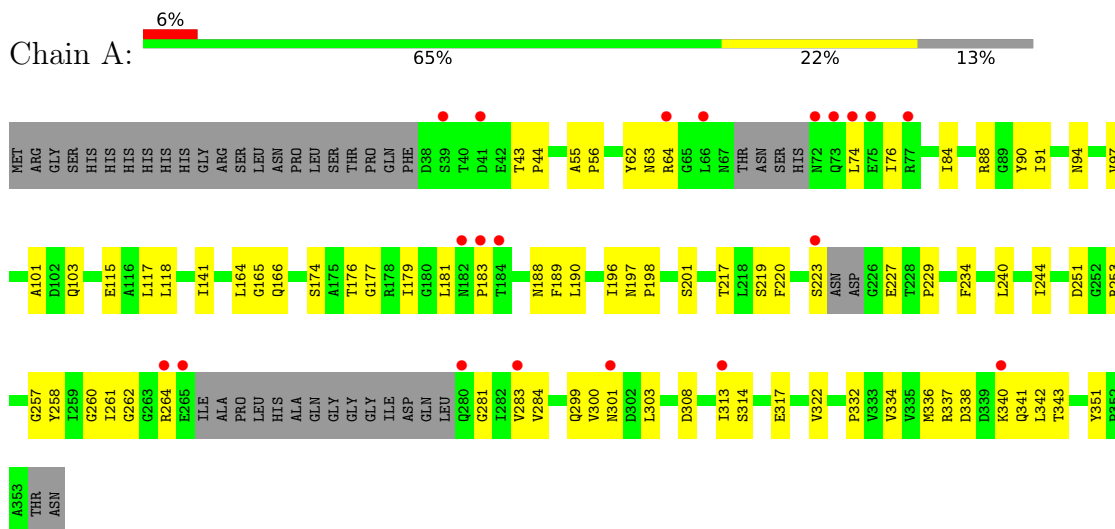
Chain A:

- Molecule 1: DegS protease

Chain B:

- Molecule 1: DegS protease

Chain C:

L138 A157 I158 T167 I168 T169 T176 I179 G180 LEU N182 P183 Q187 L190 I196 S201 S219 F220 D221 K222 SER ASN ASP GLY E227 M245 D246 K247 V254 I259 G262 I266 A267 P268 LEU HIS ALA GLN GLY GLY GLY ILE ASP Q278 L279

Q280 G281 A296 G297 I298 Q299 V300 N301 D302 L303 I304 I305 A312 L316 M319 I325 I331 P332 V335 M336 Q341 L344 Q345 V346 T347 I348 Y351 P352 A353 T354 ASN

• Molecule 2: YQF peptide

Chain D:

67%

67%   33%

Y408 Q409 F410

• Molecule 2: YQF peptide

Chain E:

100%

67%   33%

Y408 Q409 F410

• Molecule 2: YQF peptide

Chain F:

33%   67%

Y408 Q409 F410

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.88Å 172.28Å 114.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.04 – 2.49 32.04 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.9 (32.04-2.49) 95.9 (32.04-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.224 0.187 , 0.220	Depositor DCC
R_{free} test set	2003 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å²)	48.8	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 63.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6662	wwPDB-VP
Average B, all atoms (Å²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIS

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	0.24	0/2204	0.45	0/2996
1	B	0.29	0/2115	0.50	0/2881
1	C	0.27	0/2200	0.49	0/2989
2	D	0.29	0/34	0.27	0/43
2	E	0.32	0/34	0.28	0/43
2	F	0.33	0/34	0.27	0/43
All	All	0.27	0/6621	0.48	0/8995

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2193	0	2232	63	0
1	B	2103	0	2129	66	0
1	C	2189	0	2239	49	0
2	D	33	0	25	1	0
2	E	33	0	25	2	0
2	F	33	0	25	5	0
3	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	0	0	0
3	C	32	0	0	0	0
All	All	6662	0	6675	170	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 13.

The worst 5 of 170 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:261:ILE:HG13	1:B:293:ALA:HB1	1.45	0.96
1:B:181:LEU:HD21	1:B:220:PHE:CD1	2.05	0.91
1:C:87:GLN:HE22	1:C:138:LEU:H	1.16	0.90
1:B:178:ARG:O	1:B:179:ILE:HG12	1.72	0.89
1:A:179:ILE:HD12	1:A:183:PRO:HA	1.57	0.87

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	287/340 (84%)	279 (97%)	8 (3%)	0	100	100
1	B	273/340 (80%)	262 (96%)	9 (3%)	2 (1%)	22	36
1	C	283/340 (83%)	282 (100%)	1 (0%)	0	100	100
2	D	1/3 (33%)	1 (100%)	0	0	100	100
2	E	1/3 (33%)	1 (100%)	0	0	100	100
2	F	1/3 (33%)	1 (100%)	0	0	100	100
All	All	846/1029 (82%)	826 (98%)	18 (2%)	2 (0%)	47	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	179	ILE
1	B	137	GLY

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	235/275 (86%)	234 (100%)	1 (0%)	91	96
1	B	226/275 (82%)	225 (100%)	1 (0%)	91	96
1	C	234/275 (85%)	233 (100%)	1 (0%)	91	96
2	D	3/3 (100%)	3 (100%)	0	100	100
2	E	3/3 (100%)	3 (100%)	0	100	100
2	F	3/3 (100%)	3 (100%)	0	100	100
All	All	704/834 (84%)	701 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	B	179	ILE
1	C	319	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	87	GLN
1	C	278	GLN
2	F	409	GLN
1	C	295	ASN
1	A	295	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	MIS	C	201	1	11,12,13	0.70	0	10,16,18	0.78	0
1	MIS	B	201	1	11,12,13	0.73	0	10,16,18	0.72	0
1	MIS	A	201	1	11,12,13	0.67	0	10,16,18	0.68	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
1	MIS	C	201	1	-	3/10/13/15	-
1	MIS	B	201	1	-	6/10/13/15	-
1	MIS	A	201	1	-	3/10/13/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	201	MIS	CB-OG-P-O2P
1	A	201	MIS	CB-OG-P-O3P
1	B	201	MIS	CB-OG-P-O1P
1	B	201	MIS	CB-OG-P-O2P
1	B	201	MIS	CB-OG-P-O3P

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	201	MIS	5	0
1	B	201	MIS	3	0
1	A	201	MIS	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	295/340 (86%)	0.26	20 (6%)	17	17	39, 82, 143, 168	0
1	B	283/340 (83%)	0.59	46 (16%)	1	1	28, 50, 176, 198	0
1	C	293/340 (86%)	-0.01	14 (4%)	30	32	34, 54, 107, 150	0
2	D	3/3 (100%)	2.64	2 (66%)	0	0	128, 128, 139, 140	0
2	E	3/3 (100%)	3.62	3 (100%)	0	0	145, 145, 162, 164	0
2	F	3/3 (100%)	0.51	0	100	100	66, 66, 81, 99	0
All	All	880/1029 (85%)	0.29	85 (9%)	7	7	28, 60, 152, 198	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	ILE	11.3
1	B	313	ILE	8.4
1	A	66	LEU	7.0
1	B	181	LEU	6.5
1	A	74	LEU	6.4

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

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(Å²)	Q<0.9
1	MIS	B	201	13/14	0.98	0.15	26,35,60,78	0
1	MIS	A	201	13/14	0.99	0.12	40,51,60,67	0
1	MIS	C	201	13/14	0.99	0.18	30,34,46,54	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.