



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2017 – 06:03 PM EDT

PDB ID : 2QF0  
Title : Structure of the delta PDZ truncation of the DegS protease  
Authors : Sohn, J.; Grant, R.A.; Sauer, R.T.  
Deposited on : unknown  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

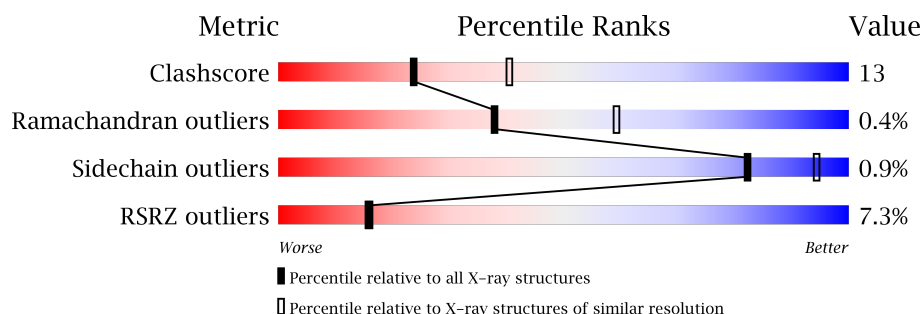
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



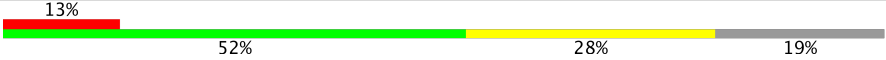

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	
1	B	243	
1	C	243	
1	D	243	
1	E	243	
1	F	243	
1	G	243	

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Mol	Chain	Length	Quality of chain
1	H	243	
1	I	243	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13852 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 Protease degS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	Se	0	0	0
			1507	941	267	296	3			
1	B	211	Total	C	N	O	Se	0	0	0
			1570	978	282	307	3			
1	C	206	Total	C	N	O	Se	0	0	0
			1533	959	275	296	3			
1	D	204	Total	C	N	O	Se	0	0	0
			1529	957	276	293	3			
1	E	193	Total	C	N	O	Se	0	0	0
			1442	905	255	279	3			
1	F	208	Total	C	N	O	Se	0	0	0
			1547	966	278	300	3			
1	G	196	Total	C	N	O	Se	0	0	0
			1460	917	260	280	3			
1	H	196	Total	C	N	O	Se	0	0	0
			1455	914	260	278	3			
1	I	189	Total	C	N	O	Se	0	0	0
			1397	877	246	271	3			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
A	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
A	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
A	17	SER	-	EXPRESSION TAG	UNP P0AEE3
A	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
A	19	HIS	-	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	GLY	-	EXPRESSION TAG	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
A	26	SER	-	EXPRESSION TAG	UNP P0AEE3
A	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
A	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
A	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
B	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
B	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
B	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
B	17	SER	-	EXPRESSION TAG	UNP P0AEE3
B	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
B	19	HIS	-	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	GLY	-	EXPRESSION TAG	UNP P0AEE3
B	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
B	26	SER	-	EXPRESSION TAG	UNP P0AEE3
B	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
B	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
B	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
C	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
C	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
C	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
C	17	SER	-	EXPRESSION TAG	UNP P0AEE3
C	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
C	19	HIS	-	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	GLY	-	EXPRESSION TAG	UNP P0AEE3
C	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
C	26	SER	-	EXPRESSION TAG	UNP P0AEE3
C	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
C	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
C	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
D	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
D	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
D	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
D	17	SER	-	EXPRESSION TAG	UNP P0AEE3
D	18	HIS	-	EXPRESSION TAG	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	HIS	-	EXPRESSION TAG	UNP P0AEE3
D	20	HIS	-	EXPRESSION TAG	UNP P0AEE3
D	21	HIS	-	EXPRESSION TAG	UNP P0AEE3
D	22	HIS	-	EXPRESSION TAG	UNP P0AEE3
D	23	HIS	-	EXPRESSION TAG	UNP P0AEE3
D	24	GLY	-	EXPRESSION TAG	UNP P0AEE3
D	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
D	26	SER	-	EXPRESSION TAG	UNP P0AEE3
D	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
D	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
D	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
E	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
E	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
E	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
E	17	SER	-	EXPRESSION TAG	UNP P0AEE3
E	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
E	19	HIS	-	EXPRESSION TAG	UNP P0AEE3
E	20	HIS	-	EXPRESSION TAG	UNP P0AEE3
E	21	HIS	-	EXPRESSION TAG	UNP P0AEE3
E	22	HIS	-	EXPRESSION TAG	UNP P0AEE3
E	23	HIS	-	EXPRESSION TAG	UNP P0AEE3
E	24	GLY	-	EXPRESSION TAG	UNP P0AEE3
E	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
E	26	SER	-	EXPRESSION TAG	UNP P0AEE3
E	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
E	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
E	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
F	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
F	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
F	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
F	17	SER	-	EXPRESSION TAG	UNP P0AEE3
F	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	19	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	20	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	21	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	22	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	23	HIS	-	EXPRESSION TAG	UNP P0AEE3
F	24	GLY	-	EXPRESSION TAG	UNP P0AEE3
F	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
F	26	SER	-	EXPRESSION TAG	UNP P0AEE3
F	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
F	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
G	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
G	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
G	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
G	17	SER	-	EXPRESSION TAG	UNP P0AEE3
G	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	19	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	20	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	21	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	22	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	23	HIS	-	EXPRESSION TAG	UNP P0AEE3
G	24	GLY	-	EXPRESSION TAG	UNP P0AEE3
G	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
G	26	SER	-	EXPRESSION TAG	UNP P0AEE3
G	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
G	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
G	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
H	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
H	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
H	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
H	17	SER	-	EXPRESSION TAG	UNP P0AEE3
H	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	19	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	20	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	21	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	22	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	23	HIS	-	EXPRESSION TAG	UNP P0AEE3
H	24	GLY	-	EXPRESSION TAG	UNP P0AEE3
H	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
H	26	SER	-	EXPRESSION TAG	UNP P0AEE3
H	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
H	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
H	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
I	14	MSE	-	EXPRESSION TAG	UNP P0AEE3
I	15	ARG	-	EXPRESSION TAG	UNP P0AEE3
I	16	GLY	-	EXPRESSION TAG	UNP P0AEE3
I	17	SER	-	EXPRESSION TAG	UNP P0AEE3
I	18	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	19	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	20	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	21	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	22	HIS	-	EXPRESSION TAG	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	23	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	24	GLY	-	EXPRESSION TAG	UNP P0AEE3
I	25	ARG	-	EXPRESSION TAG	UNP P0AEE3
I	26	SER	-	EXPRESSION TAG	UNP P0AEE3
I	85	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
I	213	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3
I	245	MSE	MET	MODIFIED RESIDUE	UNP P0AEE3

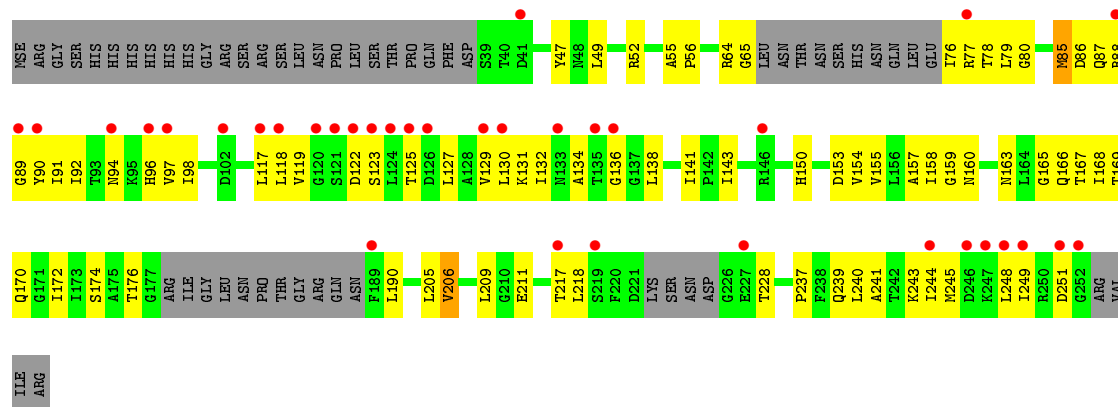
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	70	Total O 70 70	0	0
2	C	63	Total O 63 63	0	0
2	D	48	Total O 48 48	0	0
2	E	39	Total O 39 39	0	0
2	F	70	Total O 70 70	0	0
2	G	30	Total O 30 30	0	0
2	H	21	Total O 21 21	0	0
2	I	14	Total O 14 14	0	0









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.17Å 132.97Å 229.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.53 – 2.50 47.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.0 (42.53-2.50) 93.8 (47.82-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.257 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5181e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.39	0/1522	0.66	0/2061
1	B	0.40	0/1585	0.69	1/2147 (0.0%)
1	C	0.36	0/1548	0.66	0/2096
1	D	0.36	0/1544	0.64	0/2091
1	E	0.33	0/1456	0.62	0/1970
1	F	0.38	0/1562	0.68	1/2115 (0.0%)
1	G	0.33	0/1475	0.61	0/1999
1	H	0.31	0/1470	0.59	0/1991
1	I	0.29	0/1410	0.55	0/1909
All	All	0.35	0/13572	0.63	2/18379 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	79	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	136	GLY	N-CA-C	5.07	125.78	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	1507	0	1515	18	0
1	B	1570	0	1588	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1533	0	1560	31	0
1	D	1529	0	1558	39	0
1	E	1442	0	1460	27	0
1	F	1547	0	1571	38	0
1	G	1460	0	1492	36	0
1	H	1455	0	1486	67	0
1	I	1397	0	1416	71	0
2	A	57	0	0	1	0
2	B	70	0	0	1	0
2	C	63	0	0	1	0
2	D	48	0	0	1	0
2	E	39	0	0	0	0
2	F	70	0	0	0	0
2	G	30	0	0	0	0
2	H	21	0	0	0	0
2	I	14	0	0	0	0
All	All	13852	0	13646	341	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 341 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:223:SER:HB3	1:C:226:GLY:HA2	1.45	0.98
1:F:79:LEU:HD11	1:F:163:ASN:HB2	1.58	0.86
1:H:167:THR:HG23	1:I:174:SER:HB3	1.58	0.85
1:H:105:ILE:HG13	1:H:114:PHE:O	1.78	0.84
1:D:147:ARG:HD2	1:D:211:GLU:OE2	1.78	0.84

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	196/243 (81%)	190 (97%)	6 (3%)	0	100	100
1	B	205/243 (84%)	196 (96%)	7 (3%)	2 (1%)	18	32
1	C	200/243 (82%)	193 (96%)	7 (4%)	0	100	100
1	D	198/243 (82%)	187 (94%)	11 (6%)	0	100	100
1	E	185/243 (76%)	177 (96%)	8 (4%)	0	100	100
1	F	202/243 (83%)	195 (96%)	7 (4%)	0	100	100
1	G	190/243 (78%)	184 (97%)	6 (3%)	0	100	100
1	H	190/243 (78%)	168 (88%)	22 (12%)	0	100	100
1	I	181/243 (74%)	155 (86%)	21 (12%)	5 (3%)	6	8
All	All	1747/2187 (80%)	1645 (94%)	95 (5%)	7 (0%)	38	59

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	251	ASP
1	B	40	THR
1	I	206	VAL
1	I	136	GLY
1	B	67	ASN

### 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	163/196 (83%)	161 (99%)	2 (1%)	75	91
1	B	170/196 (87%)	168 (99%)	2 (1%)	75	91
1	C	165/196 (84%)	164 (99%)	1 (1%)	89	97
1	D	166/196 (85%)	165 (99%)	1 (1%)	89	97
1	E	156/196 (80%)	152 (97%)	4 (3%)	51	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	167/196 (85%)	166 (99%)	1 (1%)	89	97
1	G	158/196 (81%)	157 (99%)	1 (1%)	89	97
1	H	156/196 (80%)	155 (99%)	1 (1%)	89	97
1	I	150/196 (76%)	150 (100%)	0	100	100
All	All	1451/1764 (82%)	1438 (99%)	13 (1%)	82	94

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	117	LEU
1	E	37	PHE
1	F	239	GLN
1	C	140	THR
1	E	251	ASP

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

Mol	Chain	Res	Type
1	D	69	ASN
1	G	170	GLN
1	H	170	GLN
1	B	94	ASN
1	H	63	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	199/243 (81%)	0.24	6 (3%) 51 53	20, 37, 75, 90	0
1	B	208/243 (85%)	0.31	7 (3%) 46 48	17, 32, 76, 107	0
1	C	203/243 (83%)	0.34	14 (6%) 18 18	18, 35, 78, 94	0
1	D	201/243 (82%)	0.31	9 (4%) 34 36	20, 39, 79, 96	1 (0%)
1	E	190/243 (78%)	0.45	12 (6%) 21 21	25, 50, 83, 94	0
1	F	205/243 (84%)	0.15	6 (2%) 52 55	19, 32, 73, 86	0
1	G	193/243 (79%)	0.39	8 (4%) 38 40	29, 47, 84, 92	0
1	H	193/243 (79%)	0.80	32 (16%) 2 1	32, 62, 98, 109	0
1	I	186/243 (76%)	1.18	35 (18%) 1 1	43, 73, 108, 129	0
All	All	1778/2187 (81%)	0.46	129 (7%) 16 16	17, 44, 92, 129	1 (0%)

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	244	ILE	7.9
1	I	252	GLY	7.4
1	H	135	THR	7.3
1	C	66	LEU	6.7
1	I	251	ASP	5.6

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.