



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:04 AM UTC

PDB ID : 3LGV / pdb_00003lgv
Title : H198P mutant of the DegS-deltaPDZ protease
Authors : Sohn, J.; Grant, R.A.; Sauer, R.T.
Deposited on : 2010-01-21
Resolution : 2.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

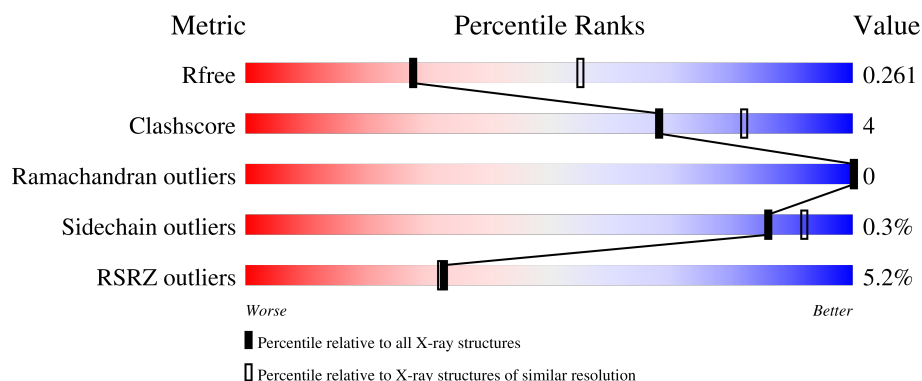
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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.



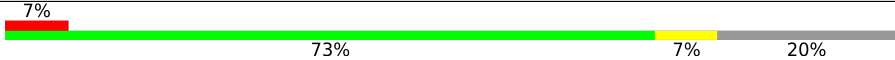
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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 $\leq 5\%$. 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	241	4% 78% 6% 15%
1	B	241	4% 78% 7% 15%
1	C	241	% 77% 7% 15%
1	D	241	6% 77% 7% 16%
1	E	241	5% 72% 9% 19%

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Mol	Chain	Length	Quality of chain
1	F	241	
1	G	241	
1	H	241	
1	I	241	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27099 atoms, of which 13516 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	204	Total	C	H	N	O	S	0	0	0
			3026	946	1518	263	296	3			
1	B	206	Total	C	H	N	O	S	0	0	0
			3079	957	1550	272	297	3			
1	C	205	Total	C	H	N	O	S	0	0	0
			3064	951	1542	272	296	3			
1	D	203	Total	C	H	N	O	S	0	0	0
			3026	942	1523	268	290	3			
1	E	195	Total	C	H	N	O	S	0	0	0
			2910	912	1463	253	279	3			
1	F	207	Total	C	H	N	O	S	0	0	0
			3069	957	1541	272	296	3			
1	G	200	Total	C	H	N	O	S	0	0	0
			2962	925	1490	258	286	3			
1	H	197	Total	C	H	N	O	S	0	0	0
			2902	907	1461	254	277	3			
1	I	193	Total	C	H	N	O	S	0	0	0
			2853	893	1428	250	279	3			

There are 108 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	198	PRO	HIS	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
B	26	GLY	-	expression tag	UNP P0AEE3
B	198	PRO	HIS	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
D	16	MET	-	expression tag	UNP P0AEE3
D	17	ARG	-	expression tag	UNP P0AEE3
D	18	GLY	-	expression tag	UNP P0AEE3
D	19	SER	-	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	HIS	-	expression tag	UNP P0AEE3
D	25	HIS	-	expression tag	UNP P0AEE3
D	26	GLY	-	expression tag	UNP P0AEE3
D	198	PRO	HIS	engineered mutation	UNP P0AEE3
E	16	MET	-	expression tag	UNP P0AEE3
E	17	ARG	-	expression tag	UNP P0AEE3
E	18	GLY	-	expression tag	UNP P0AEE3
E	19	SER	-	expression tag	UNP P0AEE3
E	20	HIS	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	21	HIS	-	expression tag	UNP P0AEE3
E	22	HIS	-	expression tag	UNP P0AEE3
E	23	HIS	-	expression tag	UNP P0AEE3
E	24	HIS	-	expression tag	UNP P0AEE3
E	25	HIS	-	expression tag	UNP P0AEE3
E	26	GLY	-	expression tag	UNP P0AEE3
E	198	PRO	HIS	engineered mutation	UNP P0AEE3
F	16	MET	-	expression tag	UNP P0AEE3
F	17	ARG	-	expression tag	UNP P0AEE3
F	18	GLY	-	expression tag	UNP P0AEE3
F	19	SER	-	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	HIS	-	expression tag	UNP P0AEE3
F	25	HIS	-	expression tag	UNP P0AEE3
F	26	GLY	-	expression tag	UNP P0AEE3
F	198	PRO	HIS	engineered mutation	UNP P0AEE3
G	16	MET	-	expression tag	UNP P0AEE3
G	17	ARG	-	expression tag	UNP P0AEE3
G	18	GLY	-	expression tag	UNP P0AEE3
G	19	SER	-	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	HIS	-	expression tag	UNP P0AEE3
G	25	HIS	-	expression tag	UNP P0AEE3
G	26	GLY	-	expression tag	UNP P0AEE3
G	198	PRO	HIS	engineered mutation	UNP P0AEE3
H	16	MET	-	expression tag	UNP P0AEE3
H	17	ARG	-	expression tag	UNP P0AEE3
H	18	GLY	-	expression tag	UNP P0AEE3
H	19	SER	-	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	HIS	-	expression tag	UNP P0AEE3
H	25	HIS	-	expression tag	UNP P0AEE3
H	26	GLY	-	expression tag	UNP P0AEE3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	198	PRO	HIS	engineered mutation	UNP P0AEE3
I	16	MET	-	expression tag	UNP P0AEE3
I	17	ARG	-	expression tag	UNP P0AEE3
I	18	GLY	-	expression tag	UNP P0AEE3
I	19	SER	-	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
I	23	HIS	-	expression tag	UNP P0AEE3
I	24	HIS	-	expression tag	UNP P0AEE3
I	25	HIS	-	expression tag	UNP P0AEE3
I	26	GLY	-	expression tag	UNP P0AEE3
I	198	PRO	HIS	engineered mutation	UNP P0AEE3

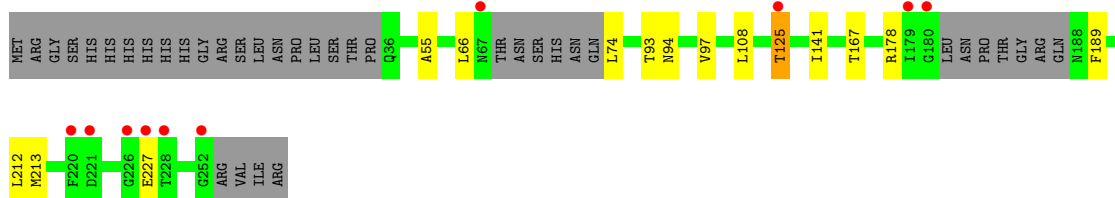
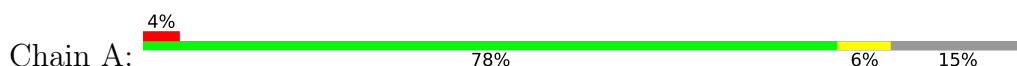
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	41	Total O 41 41	0	0
2	B	30	Total O 30 30	0	0
2	C	28	Total O 28 28	0	0
2	D	17	Total O 17 17	0	0
2	E	21	Total O 21 21	0	0
2	F	28	Total O 28 28	0	0
2	G	20	Total O 20 20	0	0
2	H	13	Total O 13 13	0	0
2	I	10	Total O 10 10	0	0

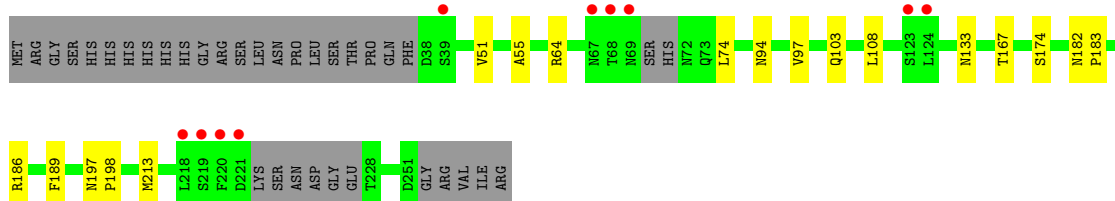
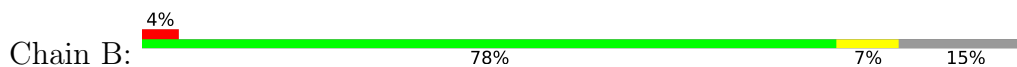
3 Residue-property plots [i](#)

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.

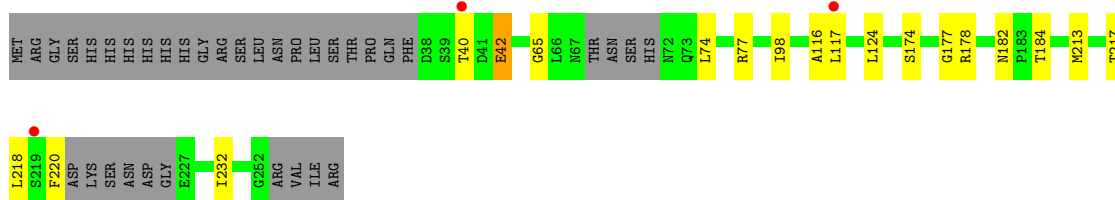
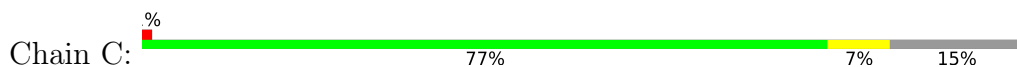
- Molecule 1: Protease degS



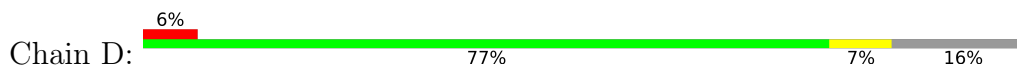
- Molecule 1: Protease degS



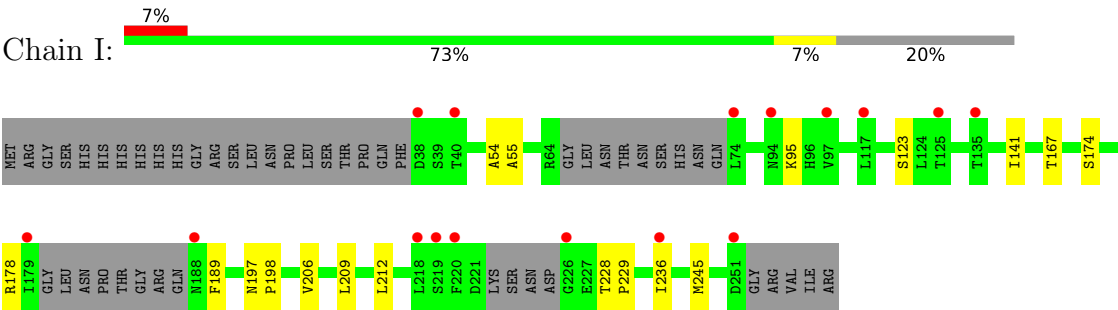
- Molecule 1: Protease degS



- Molecule 1: Protease degS



● Molecule 1: Protease degS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.54Å 133.56Å 230.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.82 – 2.73 33.82 – 2.73	Depositor EDS
% Data completeness (in resolution range)	94.1 (33.82-2.73) 94.1 (33.82-2.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.219 , 0.270 0.210 , 0.261	Depositor DCC
R_{free} test set	2856 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27099	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 43.15 % 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 1.8376e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0/1526	0.74	3/2073 (0.1%)
1	B	0.39	0/1547	0.75	0/2104
1	C	0.41	0/1540	0.72	0/2093
1	D	0.37	0/1521	0.72	0/2068
1	E	0.35	0/1464	0.70	0/1988
1	F	0.39	0/1548	0.73	0/2108
1	G	0.36	0/1490	0.72	0/2028
1	H	0.36	0/1459	0.69	0/1986
1	I	0.35	0/1441	0.77	2/1959 (0.1%)
All	All	0.38	0/13536	0.73	5/18407 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ALA	CA-C-N	-6.12	113.83	119.82
1	A	55	ALA	C-N-CA	-6.12	113.83	119.82
1	A	125	THR	CB-CA-C	-5.21	101.36	110.17
1	I	55	ALA	CA-C-N	-5.13	114.33	119.56
1	I	55	ALA	C-N-CA	-5.13	114.33	119.56

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	1508	1518	1518	10	0
1	B	1529	1550	1550	11	0
1	C	1522	1542	1541	13	0
1	D	1503	1523	1523	13	0
1	E	1447	1463	1462	15	0
1	F	1528	1541	1541	11	0
1	G	1472	1490	1490	18	0
1	H	1441	1461	1461	8	0
1	I	1425	1428	1428	11	0
2	A	41	0	0	0	0
2	B	30	0	0	0	0
2	C	28	0	0	1	0
2	D	17	0	0	2	0
2	E	21	0	0	0	0
2	F	28	0	0	0	0
2	G	20	0	0	0	0
2	H	13	0	0	0	0
2	I	10	0	0	0	0
All	All	13583	13516	13514	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 97 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:G:236:ILE:HG23	1:G:240:LEU:HD23	1.92	0.52
1:H:167:THR:HG23	1:I:174:SER:HB3	1.92	0.51
1:E:213:MET:HA	1:E:213:MET:HE2	1.93	0.50
1:G:161:PRO:HB3	1:G:197:ASN:HB2	1.92	0.50
1:I:206:VAL:HG12	1:I:212:LEU:HA	1.95	0.48

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	198/241 (82%)	194 (98%)	4 (2%)	0	100	100
1	B	200/241 (83%)	197 (98%)	3 (2%)	0	100	100
1	C	199/241 (83%)	196 (98%)	3 (2%)	0	100	100
1	D	197/241 (82%)	193 (98%)	4 (2%)	0	100	100
1	E	187/241 (78%)	181 (97%)	6 (3%)	0	100	100
1	F	203/241 (84%)	198 (98%)	5 (2%)	0	100	100
1	G	194/241 (80%)	191 (98%)	3 (2%)	0	100	100
1	H	191/241 (79%)	186 (97%)	5 (3%)	0	100	100
1	I	185/241 (77%)	177 (96%)	8 (4%)	0	100	100
All	All	1754/2169 (81%)	1713 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	162/198 (82%)	161 (99%)	1 (1%)	78	87
1	B	165/198 (83%)	164 (99%)	1 (1%)	78	87
1	C	164/198 (83%)	162 (99%)	2 (1%)	63	77
1	D	162/198 (82%)	161 (99%)	1 (1%)	78	87
1	E	155/198 (78%)	155 (100%)	0	100	100
1	F	164/198 (83%)	164 (100%)	0	100	100
1	G	158/198 (80%)	158 (100%)	0	100	100
1	H	153/198 (77%)	153 (100%)	0	100	100
1	I	152/198 (77%)	152 (100%)	0	100	100
All	All	1435/1782 (80%)	1430 (100%)	5 (0%)	86	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	THR
1	B	133	ASN
1	C	42	GLU
1	C	232	ILE
1	D	135	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	133	ASN
1	G	103	GLN
1	I	109	GLN
1	E	216	ASN
1	A	103	GLN

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 oligosaccharides 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 ⓘ

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	204/241 (84%)	0.11	10 (4%) 35 35	25, 50, 77, 90	0
1	B	206/241 (85%)	0.05	10 (4%) 35 35	27, 47, 76, 88	0
1	C	205/241 (85%)	0.04	3 (1%) 72 69	26, 51, 80, 88	0
1	D	203/241 (84%)	0.13	15 (7%) 20 20	25, 55, 77, 86	1 (0%)
1	E	195/241 (80%)	0.32	13 (6%) 24 23	35, 61, 80, 88	0
1	F	207/241 (85%)	-0.05	7 (3%) 48 46	28, 47, 78, 88	0
1	G	200/241 (82%)	0.29	9 (4%) 38 37	41, 58, 81, 88	0
1	H	197/241 (81%)	0.37	11 (5%) 30 29	44, 66, 84, 90	0
1	I	193/241 (80%)	0.62	16 (8%) 17 17	46, 71, 86, 90	0
All	All	1810/2169 (83%)	0.20	94 (5%) 33 32	25, 57, 82, 90	1 (0%)

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	ASN	8.6
1	A	180	GLY	5.3
1	A	67	ASN	5.1
1	I	188	ASN	4.7
1	B	123	SER	4.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.