



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:21 AM GMT

PDB ID : 3LGV
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
<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

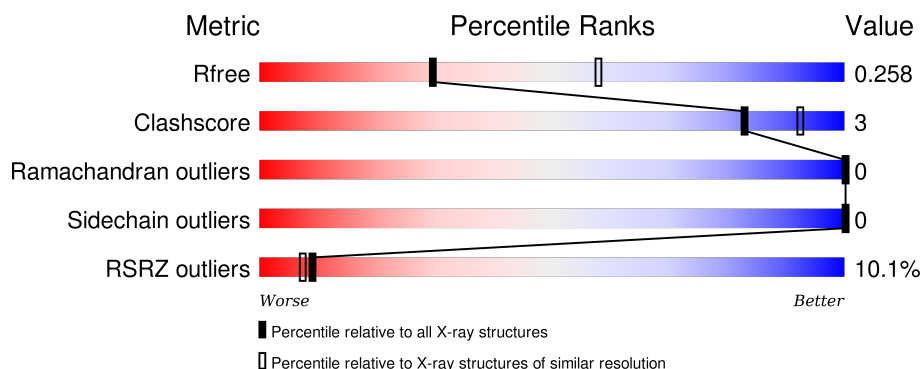
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 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	241	<div> <div>6%</div> <div>80%5%15%</div> </div>
1	B	241	<div> <div>10%</div> <div>79%7%15%</div> </div>
1	C	241	<div> <div>8%</div> <div>79%6%15%</div> </div>
1	D	241	<div> <div>10%</div> <div>78%6%16%</div> </div>
1	E	241	<div> <div>7%</div> <div>73%8%19%</div> </div>

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Mol	Chain	Length	Quality of chain		
1	F	241	5%	80%	5% 14%
1	G	241	8%	71%	12% 17%
1	H	241	10%	77%	5% 18%
1	I	241	12%	73%	7% 20%

2 Entry composition [i](#)

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	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	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	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	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	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	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	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

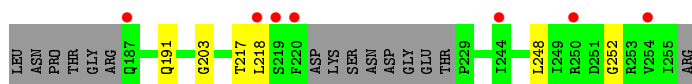
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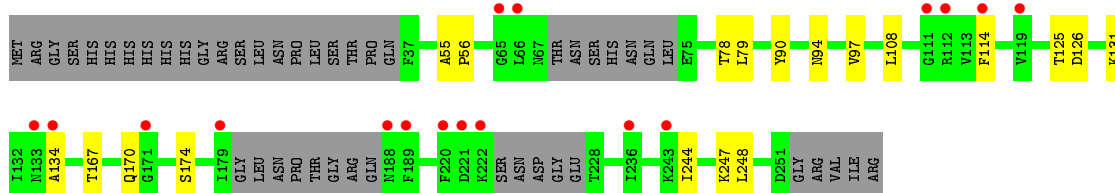
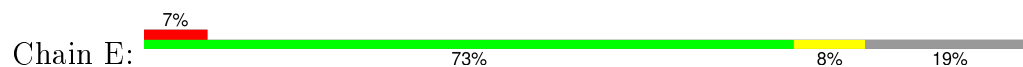
Chain	Residue	Modelled	Actual	Comment	Reference
H	198	PRO	HIS	ENGINEERED	UNP P0AEE3
I	16	MET	-	EXPRESSION TAG	UNP P0AEE3
I	17	ARG	-	EXPRESSION TAG	UNP P0AEE3
I	18	GLY	-	EXPRESSION TAG	UNP P0AEE3
I	19	SER	-	EXPRESSION TAG	UNP P0AEE3
I	20	HIS	-	EXPRESSION TAG	UNP P0AEE3
I	21	HIS	-	EXPRESSION TAG	UNP P0AEE3
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	UNP P0AEE3

- Molecule 2 is water.

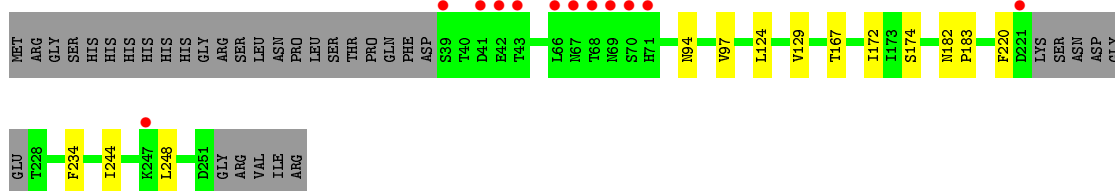
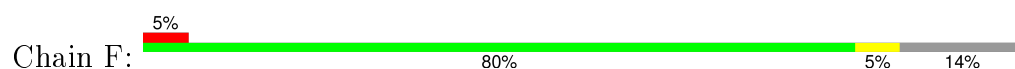
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	41	Total O 41 41	0	0
2	B	30	Total O 30 30	0	0
2	C	28	Total O 28 28	0	0
2	D	17	Total O 17 17	0	0
2	E	21	Total O 21 21	0	0
2	F	28	Total O 28 28	0	0
2	G	20	Total O 20 20	0	0
2	H	13	Total O 13 13	0	0
2	I	10	Total O 10 10	0	0



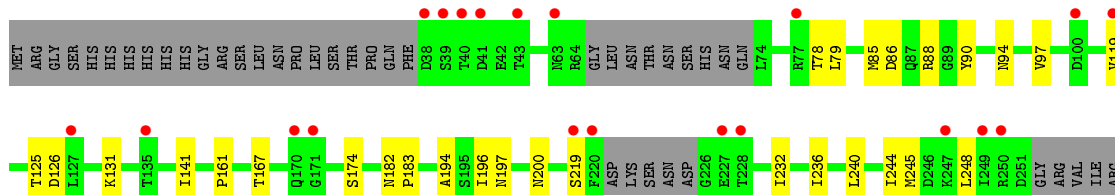
• Molecule 1: Protease degS



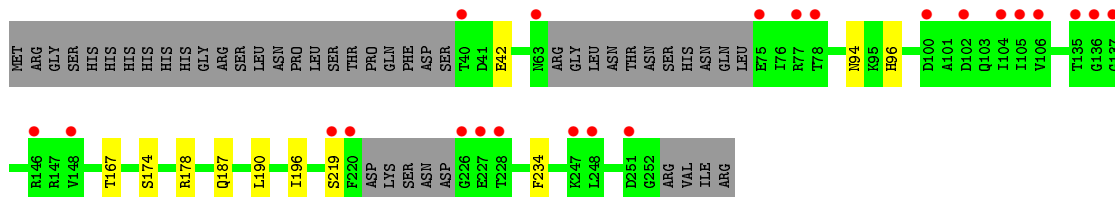
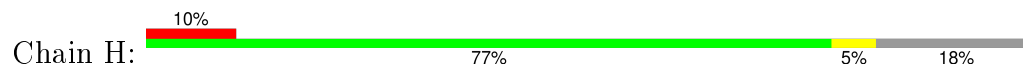
• Molecule 1: Protease degS



• Molecule 1: Protease degS

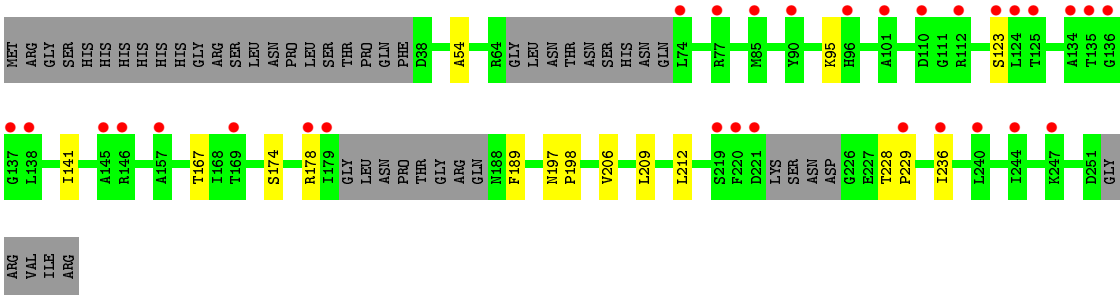


• Molecule 1: Protease degS



• 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) 94.2 (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 (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.219 , 0.270 0.204 , 0.258	Depositor DCC
R_{free} test set	2850 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 55813 reflections (0.005%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	0/1526	0.45	0/2073
1	B	0.28	0/1547	0.46	0/2104
1	C	0.29	0/1540	0.46	0/2093
1	D	0.27	0/1521	0.44	0/2068
1	E	0.27	0/1464	0.43	0/1988
1	F	0.28	0/1548	0.44	0/2108
1	G	0.27	0/1490	0.46	0/2028
1	H	0.26	0/1459	0.44	0/1986
1	I	0.26	0/1441	0.46	0/1959
All	All	0.27	0/13536	0.45	0/18407

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 [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	8	0
1	B	1529	1550	1550	10	0
1	C	1522	1542	1541	10	0
1	D	1503	1523	1523	11	0
1	E	1447	1463	1462	13	0
1	F	1528	1541	1541	9	0
1	G	1472	1490	1490	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1441	1461	1461	8	0
1	I	1425	1428	1428	10	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	83	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.

The worst 5 of 83 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: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
1:B:94:ASN:HB3	1:B:97:VAL:HG23	1.96	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	162 (100%)	0	100	100
1	B	165/198 (83%)	165 (100%)	0	100	100
1	C	164/198 (83%)	164 (100%)	0	100	100
1	D	162/198 (82%)	162 (100%)	0	100	100
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%)	1435 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	188	ASN
1	G	94	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](#)

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 [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%)	0.46	14 (6%) 20 19	24, 45, 72, 85	0
1	B	206/241 (85%)	0.46	23 (11%) 7 6	26, 44, 71, 83	0
1	C	205/241 (85%)	0.45	20 (9%) 10 8	26, 46, 74, 83	0
1	D	203/241 (84%)	0.53	23 (11%) 7 6	30, 49, 71, 81	1 (0%)
1	E	195/241 (80%)	0.58	17 (8%) 13 11	34, 56, 75, 80	0
1	F	207/241 (85%)	0.40	12 (5%) 26 26	27, 43, 71, 82	0
1	G	200/241 (82%)	0.46	20 (10%) 9 8	38, 53, 75, 81	0
1	H	197/241 (81%)	0.62	23 (11%) 6 5	42, 60, 77, 82	0
1	I	193/241 (80%)	0.91	30 (15%) 3 2	43, 64, 80, 83	0
All	All	1810/2169 (83%)	0.54	182 (10%) 9 7	24, 52, 75, 85	1 (0%)

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	125	THR	7.5
1	D	39	SER	7.4
1	F	68	THR	6.6
1	F	69	ASN	6.6
1	H	40	THR	6.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.