wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 03:55 PM JST

PDB ID	:	6JJL
Title	:	Crystal structure of the DegP dodecamer with a modulator
Authors	:	Cho, H.; Choi, Y.; Lee, H.H.; Kim, S.
Deposited on	:	2019-02-26
Resolution	:	4.20 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 (i) 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 (1)) were used in the production of this report:

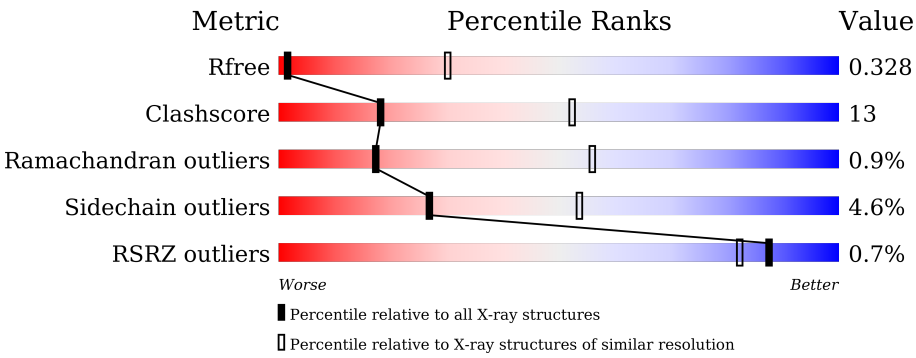
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.20 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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	440	63% 22% • 13%
1	B	440	63% 24% • 11%
1	C	440	% 58% 28% • 13%
1	D	440	2% 57% 30% • 12%
1	E	440	% 63% 24% • 12%
1	F	440	63% 22% 14%

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Mol	Chain	Length	Quality of chain
2	G	5	100%
2	H	5	80% 20%
2	I	5	80% 20%
2	J	5	100%
2	K	5	80% 20%
2	L	5	100%
2	M	5	100%
2	N	5	100%
2	O	5	100%
2	P	5	100%
2	Q	5	100%
2	R	5	100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17212 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 Periplasmic serine endoprotease DegP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2791	1741	493	544	13	0	0	0
1	B	392	2867	1783	506	565	13	0	0	0
1	C	382	2794	1742	493	546	13	0	0	0
1	D	388	2835	1766	499	557	13	0	0	0
1	E	388	2835	1765	500	557	13	0	0	0
1	F	379	2777	1733	490	541	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	SER	conflict	UNP P0C0V0
B	210	ALA	SER	conflict	UNP P0C0V0
C	210	ALA	SER	conflict	UNP P0C0V0
D	210	ALA	SER	conflict	UNP P0C0V0
E	210	ALA	SER	conflict	UNP P0C0V0
F	210	ALA	SER	conflict	UNP P0C0V0

- Molecule 2 is a protein called CYS-TYR-ARG-LYS-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	5	25	15	5	5	0	0	0
2	M	5	32	21	5	6	0	0	0
2	H	5	25	15	5	5	0	0	0

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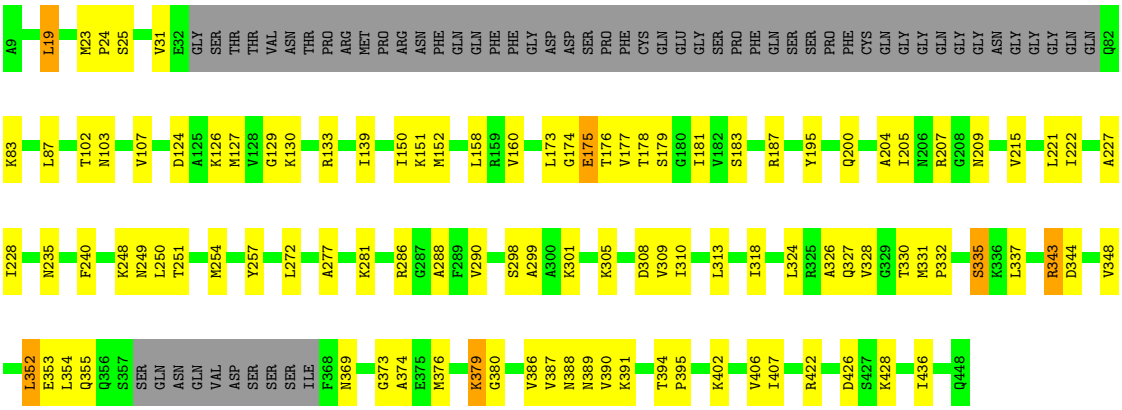
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	N	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	I	5	28	18	5	5	0	0	0
			Total	C	N	O			
2	Q	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	J	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	O	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	K	5	28	18	5	5	0	0	0
			Total	C	N	O			
2	R	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	L	5	25	15	5	5	0	0	0
			Total	C	N	O			
2	P	5	25	15	5	5	0	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.

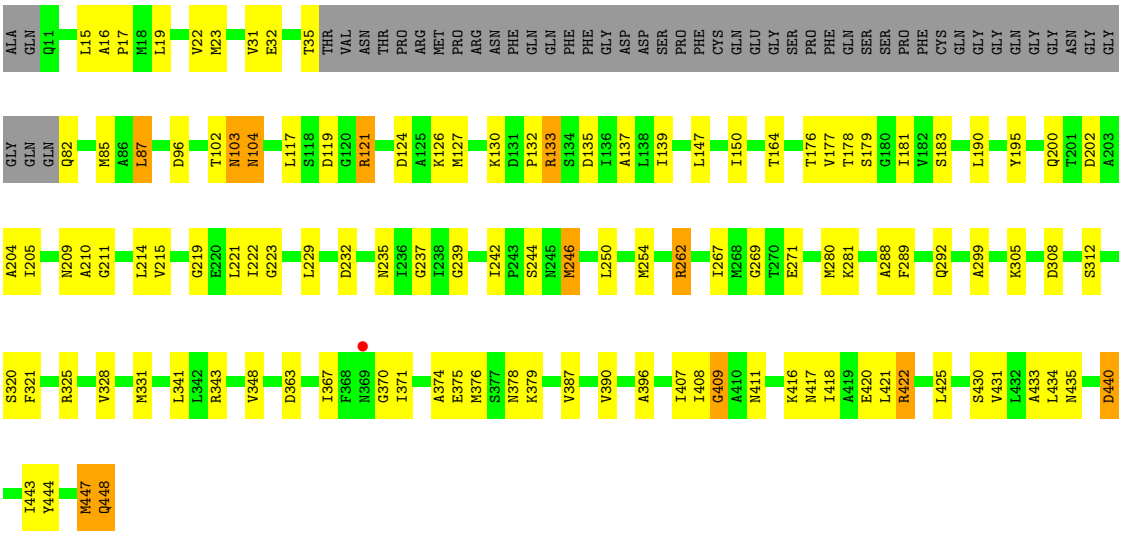
• Molecule 1: Periplasmic serine endoprotease DegP

Chain A: 63% 22% • 13%



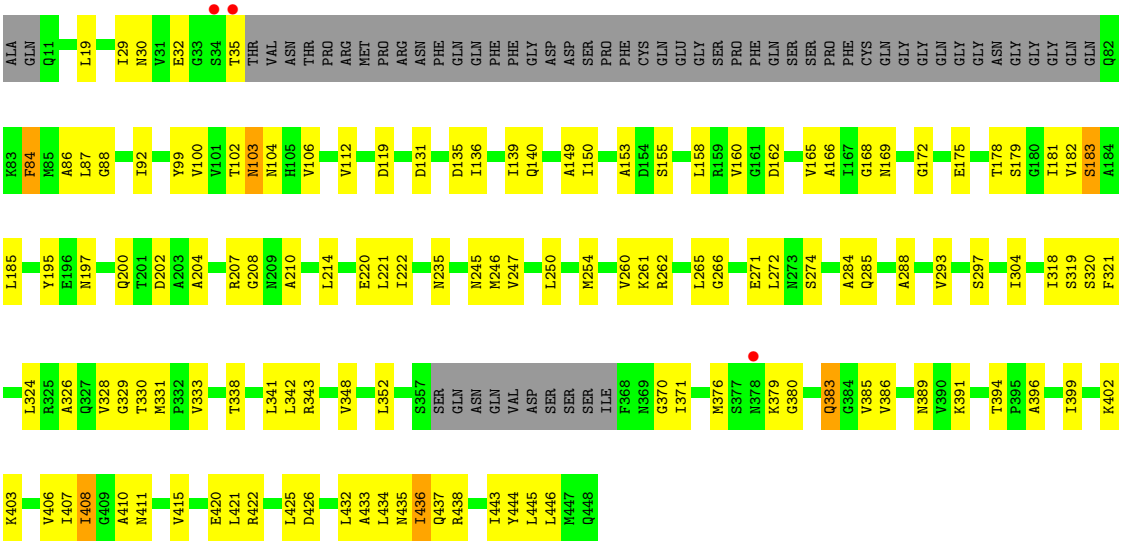
• Molecule 1: Periplasmic serine endoprotease DegP

Chain B: 63% 24% • 11%



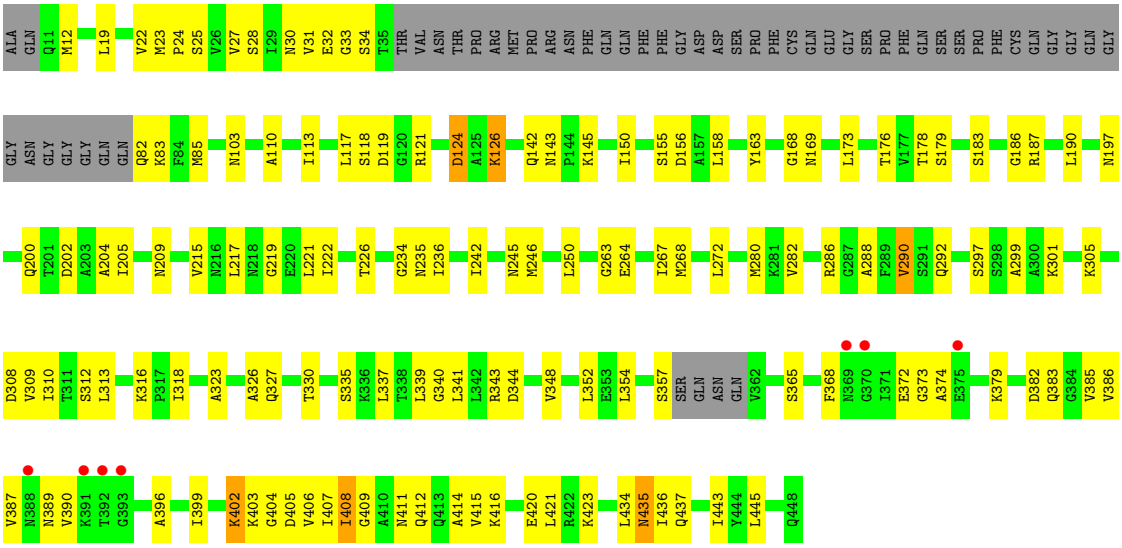
• Molecule 1: Periplasmic serine endoprotease DegP

Chain C:



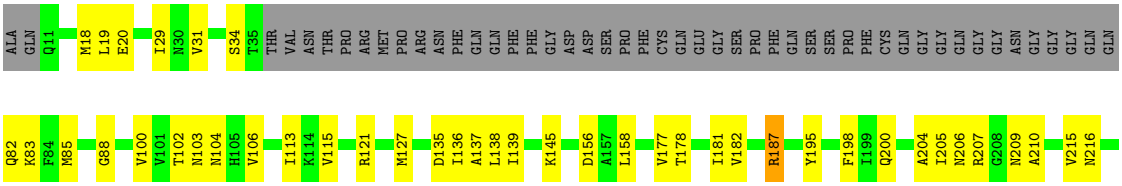
• Molecule 1: Periplasmic serine endoprotease DegP

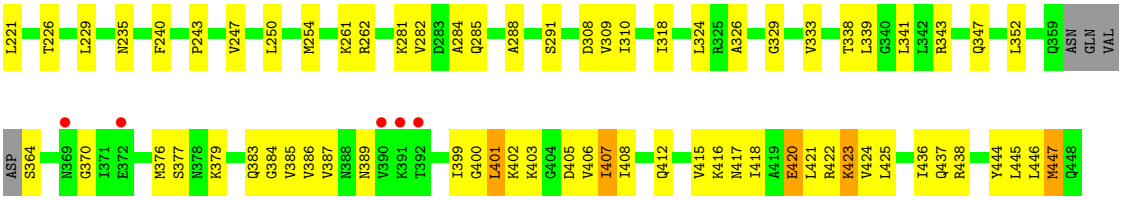
Chain D:



• Molecule 1: Periplasmic serine endoprotease DegP

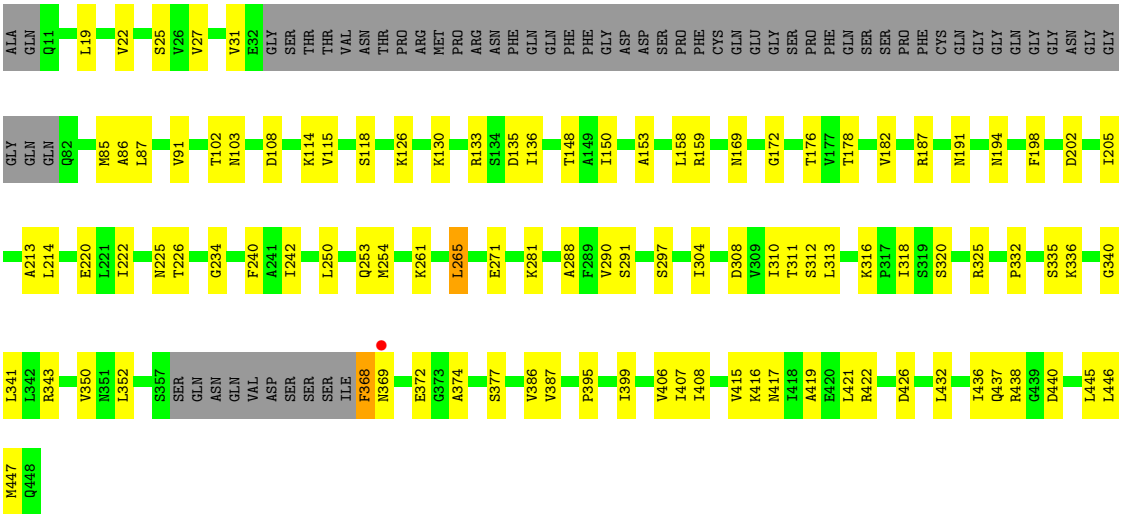
Chain E:





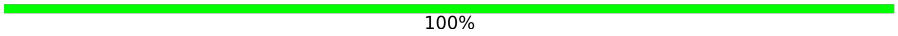
- Molecule 1: Periplasmic serine endoprotease DegP

Chain F:



- Molecule 2: CYS-TYR-ARG-LYS-LEU

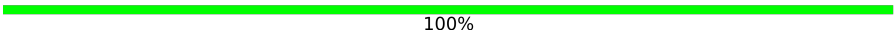
Chain G:



There are no outlier residues recorded for this chain.

- Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain M:



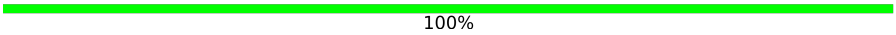
There are no outlier residues recorded for this chain.

- Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain H:

- Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain N:

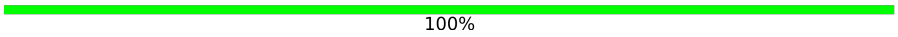


There are no outlier residues recorded for this chain.

- Molecule 2: CYS-TYR-ARG-LYS-LEU

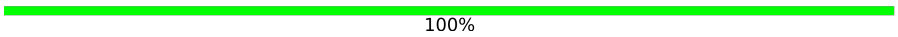
Chain I:

• Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain Q: 

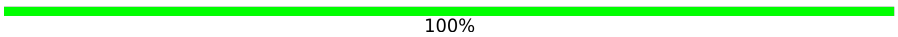
There are no outlier residues recorded for this chain.

• Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain J: 

There are no outlier residues recorded for this chain.

• Molecule 2: CYS-TYR-ARG-LYS-LEU

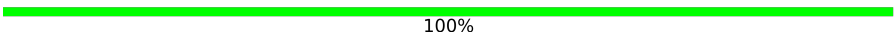
Chain O: 

There are no outlier residues recorded for this chain.

• Molecule 2: CYS-TYR-ARG-LYS-LEU

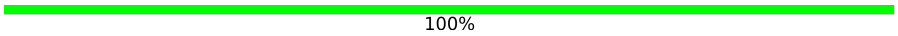
Chain K:

• Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain R: 

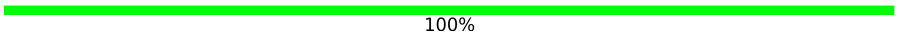
There are no outlier residues recorded for this chain.

• Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain L: 

There are no outlier residues recorded for this chain.

• Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain P: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	217.15Å 123.52Å 140.56Å 90.00° 118.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.20 40.67 – 4.16	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-4.20) 98.7 (40.67-4.16)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.248 , 0.326 0.255 , 0.328	Depositor DCC
R_{free} test set	1262 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	17212	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

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	0.35	0/2815	0.51	0/3798
1	B	0.34	0/2892	0.54	0/3904
1	C	0.37	0/2818	0.54	0/3802
1	D	0.31	0/2859	0.53	0/3858
1	E	0.32	0/2859	0.52	0/3857
1	F	0.33	0/2801	0.51	0/3779
2	G	0.58	0/24	0.44	0/32
2	H	0.42	0/24	0.39	0/32
2	I	0.37	0/27	0.69	0/36
2	J	0.41	0/24	0.39	0/32
2	K	0.37	0/27	0.66	0/36
2	L	0.35	0/24	0.43	0/32
2	M	0.36	0/32	0.42	0/43
2	N	0.35	0/24	0.28	0/32
2	O	0.33	0/24	0.32	0/32
2	P	0.26	0/24	0.30	0/32
2	Q	0.33	0/24	0.40	0/32
2	R	0.32	0/24	0.44	0/32
All	All	0.34	0/17346	0.52	0/23401

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	2791	0	2888	63	1
1	B	2867	0	2957	75	0
1	C	2794	0	2890	100	0
1	D	2835	0	2929	111	0
1	E	2835	0	2929	87	0
1	F	2777	0	2875	51	0
2	G	25	0	9	0	0
2	H	25	0	9	1	0
2	I	28	0	18	1	0
2	J	25	0	9	0	0
2	K	28	0	18	5	0
2	L	25	0	9	0	0
2	M	32	0	16	0	0
2	N	25	0	9	0	0
2	O	25	0	9	0	0
2	P	25	0	9	0	0
2	Q	25	0	9	0	0
2	R	25	0	9	0	0
All	All	17212	0	17601	466	1

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 466 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:D:387:VAL:HG21	1:D:405:ASP:H	1.14	1.10
1:D:305:LYS:HD3	1:D:343:ARG:NH2	1.84	0.93
1:E:82:GLN:HG2	1:E:83:LYS:HA	1.56	0.88
1:B:408:ILE:H	1:B:409:GLY:HA3	1.37	0.88
1:B:409:GLY:HA2	1:B:435:ASN:HB3	1.57	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:TYR:OH	1:A:257:TYR:OH[2_555]	2.05	0.15

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	375/440 (85%)	342 (91%)	28 (8%)	5 (1%)	12	48
1	B	388/440 (88%)	358 (92%)	27 (7%)	3 (1%)	19	60
1	C	376/440 (86%)	345 (92%)	29 (8%)	2 (0%)	29	68
1	D	382/440 (87%)	339 (89%)	40 (10%)	3 (1%)	19	60
1	E	382/440 (87%)	353 (92%)	25 (6%)	4 (1%)	15	54
1	F	373/440 (85%)	352 (94%)	17 (5%)	4 (1%)	14	52
2	G	3/5 (60%)	3 (100%)	0	0	100	100
2	H	3/5 (60%)	3 (100%)	0	0	100	100
2	I	3/5 (60%)	3 (100%)	0	0	100	100
2	J	3/5 (60%)	3 (100%)	0	0	100	100
2	K	3/5 (60%)	3 (100%)	0	0	100	100
2	L	3/5 (60%)	3 (100%)	0	0	100	100
2	M	3/5 (60%)	3 (100%)	0	0	100	100
2	N	3/5 (60%)	3 (100%)	0	0	100	100
2	O	3/5 (60%)	3 (100%)	0	0	100	100
2	P	3/5 (60%)	3 (100%)	0	0	100	100
2	Q	3/5 (60%)	3 (100%)	0	0	100	100
2	R	3/5 (60%)	3 (100%)	0	0	100	100
All	All	2312/2700 (86%)	2125 (92%)	166 (7%)	21 (1%)	17	56

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	408	ILE
1	F	291	SER
1	F	369	ASN
1	A	335	SER

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Mol	Chain	Res	Type
1	C	436	ILE

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	301/350 (86%)	286 (95%)	15 (5%)	24	51
1	B	312/350 (89%)	291 (93%)	21 (7%)	16	43
1	C	302/350 (86%)	293 (97%)	9 (3%)	41	63
1	D	308/350 (88%)	298 (97%)	10 (3%)	39	62
1	E	308/350 (88%)	295 (96%)	13 (4%)	30	55
1	F	300/350 (86%)	286 (95%)	14 (5%)	26	53
2	I	1/5 (20%)	0	1 (100%)	0	0
2	K	1/5 (20%)	0	1 (100%)	0	0
2	M	1/5 (20%)	1 (100%)	0	100	100
All	All	1834/2115 (87%)	1750 (95%)	84 (5%)	27	54

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	187	ARG
1	F	133	ARG
1	E	291	SER
1	E	444	TYR
1	F	297	SER

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	C	169	ASN
1	C	435	ASN
1	D	417	ASN

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Mol	Chain	Res	Type
1	B	104	ASN
1	A	355	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 monosaccharides 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	381/440 (86%)	-0.35	0	100	100	2, 30, 97, 131	0
1	B	392/440 (89%)	-0.35	1 (0%)	94	90	4, 50, 117, 166	0
1	C	382/440 (86%)	-0.29	3 (0%)	86	79	2, 29, 128, 152	0
1	D	388/440 (88%)	-0.14	7 (1%)	68	59	8, 69, 164, 208	0
1	E	388/440 (88%)	-0.21	5 (1%)	77	68	6, 55, 134, 165	0
1	F	379/440 (86%)	-0.35	1 (0%)	94	90	7, 35, 90, 119	0
2	G	5/5 (100%)	-0.30	0	100	100	24, 43, 44, 47	0
2	H	5/5 (100%)	-0.02	0	100	100	59, 67, 80, 85	0
2	I	5/5 (100%)	-0.19	0	100	100	24, 57, 76, 85	0
2	J	5/5 (100%)	-0.12	0	100	100	42, 60, 70, 73	0
2	K	5/5 (100%)	-0.11	0	100	100	60, 67, 79, 87	0
2	L	5/5 (100%)	0.24	0	100	100	57, 80, 100, 104	0
2	M	5/5 (100%)	-0.63	0	100	100	26, 33, 59, 59	0
2	N	5/5 (100%)	-0.68	0	100	100	54, 65, 70, 72	0
2	O	5/5 (100%)	0.28	0	100	100	82, 85, 107, 113	0
2	P	5/5 (100%)	0.01	0	100	100	50, 71, 90, 98	0
2	Q	5/5 (100%)	-0.20	0	100	100	28, 42, 87, 94	0
2	R	5/5 (100%)	-0.26	0	100	100	61, 65, 79, 90	0
All	All	2370/2700 (87%)	-0.28	17 (0%)	87	82	2, 45, 124, 208	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	372	GLU	4.2
1	D	393	GLY	3.6
1	E	392	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	34	SER	3.3
1	D	391	LYS	3.2

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 monosaccharides 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.