



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2022 – 12:15 PM JST

PDB ID : 7F7I
Title : Stapled Peptide Inhibitor in complex with PSD95 GK domain
Authors : Shang, Y.; Huang, X.; Li, X.; Zhang, M.
Deposited on : 2021-06-29
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

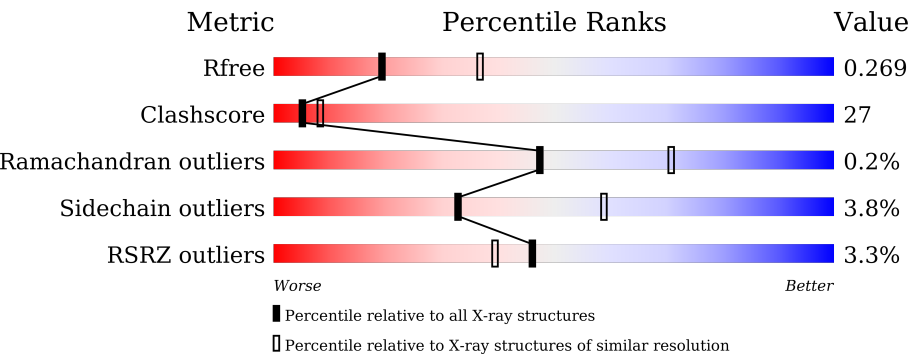
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	205	<div><div></div><div>50%37%•11%</div></div>
1	B	205	<div><div></div><div>61%31%•7%</div></div>
1	C	205	<div><div></div><div>59%28%•11%</div></div>
1	D	205	<div><div>7%</div><div>59%29%•11%</div></div>
1	E	205	<div><div>7%</div><div>47%38%•11%</div></div>
1	F	205	<div><div>7%</div><div>51%37%•11%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	14	<div><div></div><div>21%79%</div></div>
2	H	14	<div><div></div><div>64%36%</div></div>
2	I	14	<div><div></div><div>43%50%7%</div></div>
2	J	14	<div><div></div><div>21%43%57%</div></div>
2	K	14	<div><div></div><div>14%29%57%14%</div></div>
2	L	14	<div><div></div><div>14%29%50%21%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9802 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 Disks large homolog 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1469	921	265	279	4			
1	B	191	Total	C	N	O	S	0	0	0
			1512	949	269	290	4			
1	C	182	Total	C	N	O	S	0	0	0
			1453	911	262	276	4			
1	D	182	Total	C	N	O	S	1	0	0
			1460	915	263	278	4			
1	E	182	Total	C	N	O	S	0	0	0
			1429	898	253	274	4			
1	F	182	Total	C	N	O	S	0	0	0
			1445	906	261	274	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	509	MET	-	initiating methionine	UNP P31016
A	510	HIS	-	expression tag	UNP P31016
A	511	HIS	-	expression tag	UNP P31016
A	512	HIS	-	expression tag	UNP P31016
A	513	HIS	-	expression tag	UNP P31016
A	514	HIS	-	expression tag	UNP P31016
A	515	HIS	-	expression tag	UNP P31016
A	516	SER	-	expression tag	UNP P31016
A	517	SER	-	expression tag	UNP P31016
A	518	GLY	-	expression tag	UNP P31016
A	519	LEU	-	expression tag	UNP P31016
A	520	GLU	-	expression tag	UNP P31016
A	521	VAL	-	expression tag	UNP P31016
A	522	LEU	-	expression tag	UNP P31016
A	523	PHE	-	expression tag	UNP P31016
A	524	GLN	-	expression tag	UNP P31016
A	525	GLY	-	expression tag	UNP P31016

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	PRO	-	expression tag	UNP P31016
A	527	GLY	-	expression tag	UNP P31016
A	528	SER	-	expression tag	UNP P31016
A	529	GLU	-	expression tag	UNP P31016
A	530	PHE	-	expression tag	UNP P31016
B	509	MET	-	initiating methionine	UNP P31016
B	510	HIS	-	expression tag	UNP P31016
B	511	HIS	-	expression tag	UNP P31016
B	512	HIS	-	expression tag	UNP P31016
B	513	HIS	-	expression tag	UNP P31016
B	514	HIS	-	expression tag	UNP P31016
B	515	HIS	-	expression tag	UNP P31016
B	516	SER	-	expression tag	UNP P31016
B	517	SER	-	expression tag	UNP P31016
B	518	GLY	-	expression tag	UNP P31016
B	519	LEU	-	expression tag	UNP P31016
B	520	GLU	-	expression tag	UNP P31016
B	521	VAL	-	expression tag	UNP P31016
B	522	LEU	-	expression tag	UNP P31016
B	523	PHE	-	expression tag	UNP P31016
B	524	GLN	-	expression tag	UNP P31016
B	525	GLY	-	expression tag	UNP P31016
B	526	PRO	-	expression tag	UNP P31016
B	527	GLY	-	expression tag	UNP P31016
B	528	SER	-	expression tag	UNP P31016
B	529	GLU	-	expression tag	UNP P31016
B	530	PHE	-	expression tag	UNP P31016
C	509	MET	-	initiating methionine	UNP P31016
C	510	HIS	-	expression tag	UNP P31016
C	511	HIS	-	expression tag	UNP P31016
C	512	HIS	-	expression tag	UNP P31016
C	513	HIS	-	expression tag	UNP P31016
C	514	HIS	-	expression tag	UNP P31016
C	515	HIS	-	expression tag	UNP P31016
C	516	SER	-	expression tag	UNP P31016
C	517	SER	-	expression tag	UNP P31016
C	518	GLY	-	expression tag	UNP P31016
C	519	LEU	-	expression tag	UNP P31016
C	520	GLU	-	expression tag	UNP P31016
C	521	VAL	-	expression tag	UNP P31016
C	522	LEU	-	expression tag	UNP P31016
C	523	PHE	-	expression tag	UNP P31016

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	524	GLN	-	expression tag	UNP P31016
C	525	GLY	-	expression tag	UNP P31016
C	526	PRO	-	expression tag	UNP P31016
C	527	GLY	-	expression tag	UNP P31016
C	528	SER	-	expression tag	UNP P31016
C	529	GLU	-	expression tag	UNP P31016
C	530	PHE	-	expression tag	UNP P31016
D	509	MET	-	initiating methionine	UNP P31016
D	510	HIS	-	expression tag	UNP P31016
D	511	HIS	-	expression tag	UNP P31016
D	512	HIS	-	expression tag	UNP P31016
D	513	HIS	-	expression tag	UNP P31016
D	514	HIS	-	expression tag	UNP P31016
D	515	HIS	-	expression tag	UNP P31016
D	516	SER	-	expression tag	UNP P31016
D	517	SER	-	expression tag	UNP P31016
D	518	GLY	-	expression tag	UNP P31016
D	519	LEU	-	expression tag	UNP P31016
D	520	GLU	-	expression tag	UNP P31016
D	521	VAL	-	expression tag	UNP P31016
D	522	LEU	-	expression tag	UNP P31016
D	523	PHE	-	expression tag	UNP P31016
D	524	GLN	-	expression tag	UNP P31016
D	525	GLY	-	expression tag	UNP P31016
D	526	PRO	-	expression tag	UNP P31016
D	527	GLY	-	expression tag	UNP P31016
D	528	SER	-	expression tag	UNP P31016
D	529	GLU	-	expression tag	UNP P31016
D	530	PHE	-	expression tag	UNP P31016
E	509	MET	-	initiating methionine	UNP P31016
E	510	HIS	-	expression tag	UNP P31016
E	511	HIS	-	expression tag	UNP P31016
E	512	HIS	-	expression tag	UNP P31016
E	513	HIS	-	expression tag	UNP P31016
E	514	HIS	-	expression tag	UNP P31016
E	515	HIS	-	expression tag	UNP P31016
E	516	SER	-	expression tag	UNP P31016
E	517	SER	-	expression tag	UNP P31016
E	518	GLY	-	expression tag	UNP P31016
E	519	LEU	-	expression tag	UNP P31016
E	520	GLU	-	expression tag	UNP P31016
E	521	VAL	-	expression tag	UNP P31016

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	522	LEU	-	expression tag	UNP P31016
E	523	PHE	-	expression tag	UNP P31016
E	524	GLN	-	expression tag	UNP P31016
E	525	GLY	-	expression tag	UNP P31016
E	526	PRO	-	expression tag	UNP P31016
E	527	GLY	-	expression tag	UNP P31016
E	528	SER	-	expression tag	UNP P31016
E	529	GLU	-	expression tag	UNP P31016
E	530	PHE	-	expression tag	UNP P31016
F	509	MET	-	initiating methionine	UNP P31016
F	510	HIS	-	expression tag	UNP P31016
F	511	HIS	-	expression tag	UNP P31016
F	512	HIS	-	expression tag	UNP P31016
F	513	HIS	-	expression tag	UNP P31016
F	514	HIS	-	expression tag	UNP P31016
F	515	HIS	-	expression tag	UNP P31016
F	516	SER	-	expression tag	UNP P31016
F	517	SER	-	expression tag	UNP P31016
F	518	GLY	-	expression tag	UNP P31016
F	519	LEU	-	expression tag	UNP P31016
F	520	GLU	-	expression tag	UNP P31016
F	521	VAL	-	expression tag	UNP P31016
F	522	LEU	-	expression tag	UNP P31016
F	523	PHE	-	expression tag	UNP P31016
F	524	GLN	-	expression tag	UNP P31016
F	525	GLY	-	expression tag	UNP P31016
F	526	PRO	-	expression tag	UNP P31016
F	527	GLY	-	expression tag	UNP P31016
F	528	SER	-	expression tag	UNP P31016
F	529	GLU	-	expression tag	UNP P31016
F	530	PHE	-	expression tag	UNP P31016

- Molecule 2 is a protein called ACE-ARG-ILE-ARG-ARG-ASP-GLU-TYR-LEU-LYZ-ALA-ILE-GLN-NH₂.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	14	Total	C	N	O	0	0	1
			113	70	24	19			
2	H	14	Total	C	N	O	0	0	1
			101	64	18	19			
2	I	14	Total	C	N	O	0	0	1
			113	70	24	19			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	14	Total	C	N	O	0	0	1
			113	70	24	19			
2	K	14	Total	C	N	O	0	0	1
			107	67	21	19			
2	L	14	Total	C	N	O	0	0	1
			107	67	21	19			

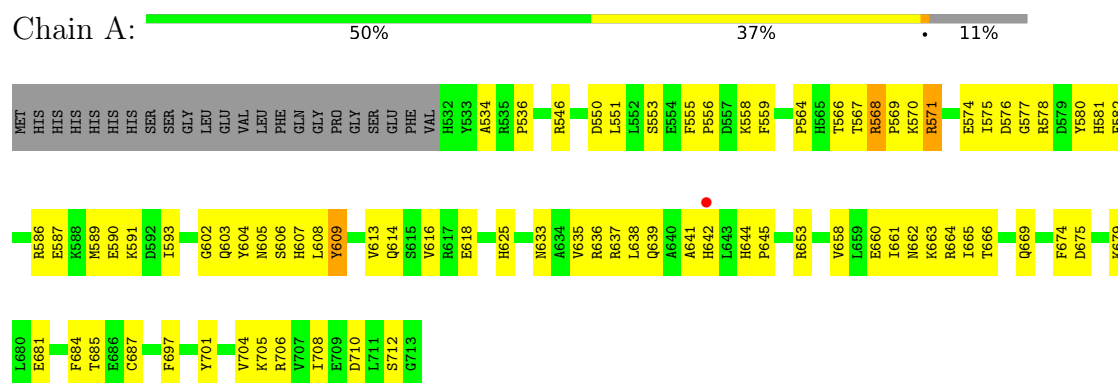
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total	O	0	0
			84	84		
3	B	77	Total	O	0	0
			77	77		
3	C	75	Total	O	0	0
			75	75		
3	D	54	Total	O	0	0
			54	54		
3	E	35	Total	O	0	0
			35	35		
3	F	37	Total	O	0	0
			37	37		
3	G	6	Total	O	0	0
			6	6		
3	H	4	Total	O	0	0
			4	4		
3	I	2	Total	O	0	0
			2	2		
3	J	1	Total	O	0	0
			1	1		
3	K	4	Total	O	0	0
			4	4		
3	L	1	Total	O	0	0
			1	1		

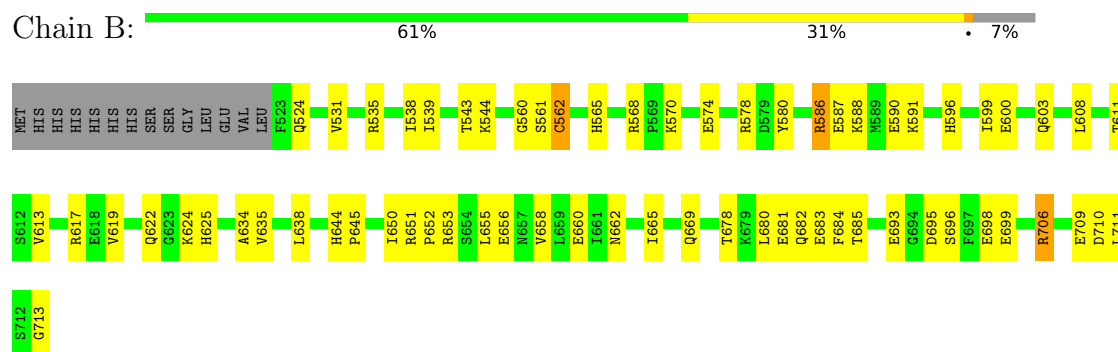
3 Residue-property plots

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.

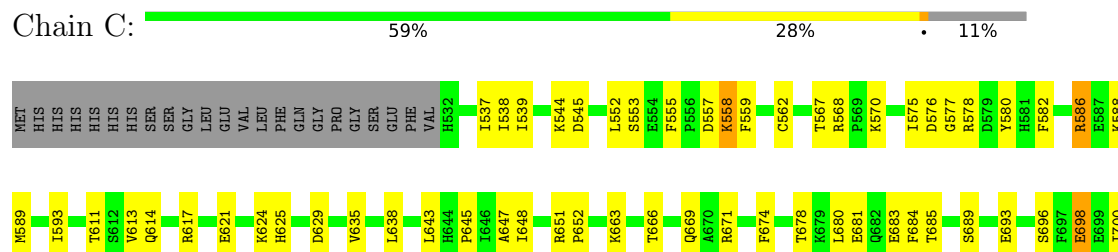
• Molecule 1: Disks large homolog 4



• Molecule 1: Disks large homolog 4



• Molecule 1: Disks large homolog 4

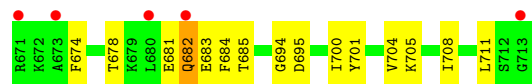
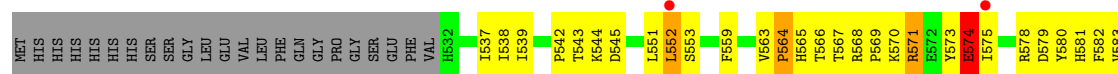




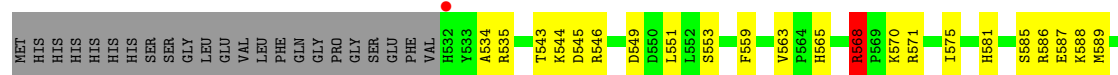
- Molecule 1: Disks large homolog 4



- Molecule 1: Disks large homolog 4

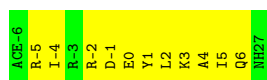


- Molecule 1: Disks large homolog 4



- Molecule 2: ACE-ARG-ILE-ARG-ARG-ASP-GLU-TYR-LEU-LYZ-ALA-ILE-GLN-NH2





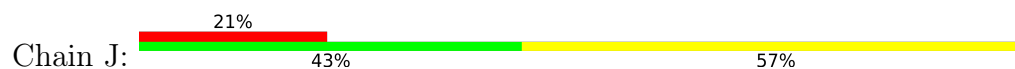
- Molecule 2: ACE-ARG-ILE-ARG-ARG-ASP-GLU-TYR-LEU-LYZ-ALA-ILE-GLN-NH2



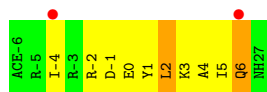
- Molecule 2: ACE-ARG-ILE-ARG-ARG-ASP-GLU-TYR-LEU-LYZ-ALA-ILE-GLN-NH2



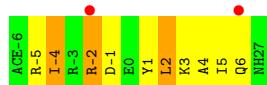
- Molecule 2: ACE-ARG-ILE-ARG-ARG-ASP-GLU-TYR-LEU-LYZ-ALA-ILE-GLN-NH2



- Molecule 2: ACE-ARG-ILE-ARG-ARG-ASP-GLU-TYR-LEU-LYZ-ALA-ILE-GLN-NH2



- Molecule 2: ACE-ARG-ILE-ARG-ARG-ASP-GLU-TYR-LEU-LYZ-ALA-ILE-GLN-NH2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.03Å 51.95Å 144.50Å 91.78° 91.43° 120.97°	Depositor
Resolution (Å)	33.52 – 2.60 33.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (33.52-2.60) 96.6 (33.52-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.214 , 0.262 0.220 , 0.269	Depositor DCC
R_{free} test set	1907 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
Reported twinning fraction	0.070 for -k,-h,-l	Depositor
Outliers	0 of 37951 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9802	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, LYZ, NH2

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	0.48	1/1499 (0.1%)	0.64	2/2021 (0.1%)
1	B	0.41	0/1543	0.64	1/2084 (0.0%)
1	C	0.44	1/1483 (0.1%)	0.66	0/2003
1	D	0.41	0/1490	0.65	0/2011
1	E	0.43	1/1458 (0.1%)	0.68	2/1973 (0.1%)
1	F	0.47	0/1475	0.69	1/1994 (0.1%)
2	G	0.25	0/99	0.42	0/129
2	H	0.22	0/87	1.47	3/115 (2.6%)
2	I	0.19	0/99	0.32	0/129
2	J	0.19	0/99	0.31	0/129
2	K	0.28	0/93	0.46	0/122
2	L	0.70	0/93	0.74	0/122
All	All	0.44	3/9518 (0.0%)	0.66	9/12832 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	564	PRO	N-CD	5.50	1.55	1.47
1	C	562	CYS	CB-SG	-5.47	1.72	1.81
1	A	569	PRO	N-CD	5.14	1.55	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	-3	ARG	O-C-N	-10.51	105.88	122.70
1	E	552	LEU	CB-CG-CD2	-10.46	93.22	111.00
2	H	-3	ARG	C-N-CA	8.64	143.31	121.70
2	H	-3	ARG	CA-C-N	7.21	133.06	117.20
1	A	644	HIS	C-N-CD	5.97	140.94	128.40

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	1469	0	1431	81	1
1	B	1512	0	1452	53	0
1	C	1453	0	1399	60	0
1	D	1460	0	1405	69	5
1	E	1429	0	1359	128	1
1	F	1445	0	1381	84	6
2	G	113	0	116	12	0
2	H	101	0	94	5	0
2	I	113	0	116	20	0
2	J	113	0	116	11	1
2	K	107	0	105	19	0
2	L	107	0	105	16	0
3	A	84	0	0	8	0
3	B	77	0	0	4	0
3	C	75	0	0	1	0
3	D	54	0	0	4	0
3	E	35	0	0	5	0
3	F	37	0	0	4	0
3	G	6	0	0	0	0
3	H	4	0	0	0	0
3	I	2	0	0	0	0
3	J	1	0	0	0	0
3	K	4	0	0	1	0
3	L	1	0	0	0	0
All	All	9802	0	9079	497	7

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 27.

The worst 5 of 497 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:F:666:THR:CG2	1:F:669:GLN:HG3	1.59	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:THR:OG1	1:D:669:GLN:CD	1.83	1.16
1:F:666:THR:HG22	1:F:669:GLN:CG	1.74	1.15
1:E:539:ILE:HG23	1:E:544:LYS:HB2	1.34	1.09
1:F:659:LEU:HD12	1:F:665:ILE:HG12	1.32	1.07

The worst 5 of 7 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:D:664:ARG:NH1	1:F:660:GLU:CD[1_455]	1.30	0.90
1:D:664:ARG:NH1	1:F:660:GLU:OE1[1_455]	1.76	0.44
1:D:664:ARG:NH2	1:F:660:GLU:OE1[1_455]	1.96	0.24
1:D:664:ARG:CZ	1:F:660:GLU:OE1[1_455]	1.99	0.21
1:A:603:GLN:NE2	2:J:6:GLN:O[1_665]	2.01	0.19

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	180/205 (88%)	174 (97%)	6 (3%)	0	100	100
1	B	189/205 (92%)	184 (97%)	5 (3%)	0	100	100
1	C	180/205 (88%)	172 (96%)	8 (4%)	0	100	100
1	D	180/205 (88%)	178 (99%)	2 (1%)	0	100	100
1	E	180/205 (88%)	173 (96%)	6 (3%)	1 (1%)	25	47
1	F	180/205 (88%)	175 (97%)	5 (3%)	0	100	100
2	G	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
2	H	11/14 (79%)	11 (100%)	0	0	100	100
2	I	11/14 (79%)	11 (100%)	0	0	100	100
2	J	11/14 (79%)	11 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	11/14 (79%)	10 (91%)	1 (9%)	0	100	100
2	L	11/14 (79%)	6 (54%)	4 (36%)	1 (9%)	1	0
All	All	1155/1314 (88%)	1115 (96%)	38 (3%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	574	GLU
2	L	-4	ILE

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	158/180 (88%)	155 (98%)	3 (2%)	57	79
1	B	160/180 (89%)	155 (97%)	5 (3%)	40	66
1	C	154/180 (86%)	148 (96%)	6 (4%)	32	58
1	D	155/180 (86%)	151 (97%)	4 (3%)	46	72
1	E	149/180 (83%)	143 (96%)	6 (4%)	31	57
1	F	152/180 (84%)	146 (96%)	6 (4%)	32	58
2	G	10/10 (100%)	8 (80%)	2 (20%)	1	2
2	H	8/10 (80%)	8 (100%)	0	100	100
2	I	10/10 (100%)	9 (90%)	1 (10%)	7	14
2	J	10/10 (100%)	10 (100%)	0	100	100
2	K	9/10 (90%)	7 (78%)	2 (22%)	1	1
2	L	9/10 (90%)	7 (78%)	2 (22%)	1	1
All	All	984/1140 (86%)	947 (96%)	37 (4%)	33	59

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	675	ASP
2	L	-2	ARG
1	F	676	ARG
2	I	0	GLU
1	C	698	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	605	ASN
1	E	614	GLN
2	L	6	GLN
1	E	657	ASN
1	E	607	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
2	LYZ	L	3	2	7,9,10	0.72	0	4,10,12	0.75	0
2	LYZ	H	3	2	7,9,10	0.72	0	4,10,12	0.72	0
2	LYZ	J	3	2	7,9,10	0.73	0	4,10,12	0.78	0
2	LYZ	G	3	2	7,9,10	0.72	0	4,10,12	0.68	0
2	LYZ	K	3	2	7,9,10	0.73	0	4,10,12	0.69	0
2	LYZ	I	3	2	7,9,10	0.73	0	4,10,12	0.77	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
2	LYZ	L	3	2	-	0/8/9/11	-
2	LYZ	H	3	2	-	3/8/9/11	-
2	LYZ	J	3	2	-	4/8/9/11	-
2	LYZ	G	3	2	-	0/8/9/11	-
2	LYZ	K	3	2	-	0/8/9/11	-
2	LYZ	I	3	2	-	5/8/9/11	-

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
2	H	3	LYZ	OH-CD-CE-NZ
2	I	3	LYZ	OH-CD-CG-CB
2	I	3	LYZ	CG-CD-CE-NZ
2	I	3	LYZ	OH-CD-CE-NZ
2	J	3	LYZ	OH-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	3	LYZ	1	0
2	G	3	LYZ	1	0
2	K	3	LYZ	1	0

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	182/205 (88%)	-0.11	1 (0%) 91 89	25, 39, 59, 117	0
1	B	191/205 (93%)	-0.20	0 100 100	24, 37, 65, 84	0
1	C	182/205 (88%)	-0.18	0 100 100	21, 37, 58, 72	0
1	D	182/205 (88%)	-0.14	2 (1%) 80 78	23, 40, 63, 87	2 (1%)
1	E	182/205 (88%)	0.43	14 (7%) 13 10	35, 61, 106, 127	0
1	F	182/205 (88%)	0.36	14 (7%) 13 10	29, 58, 105, 128	1 (0%)
2	G	11/14 (78%)	-0.31	0 100 100	33, 42, 55, 61	0
2	H	11/14 (78%)	0.33	0 100 100	29, 45, 81, 82	0
2	I	11/14 (78%)	-0.04	0 100 100	28, 45, 53, 63	0
2	J	11/14 (78%)	0.65	3 (27%) 0 0	37, 45, 80, 90	0
2	K	11/14 (78%)	0.84	2 (18%) 1 0	48, 67, 107, 108	0
2	L	11/14 (78%)	0.90	2 (18%) 1 0	37, 64, 93, 93	0
All	All	1167/1314 (88%)	0.05	38 (3%) 46 39	21, 45, 92, 128	3 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	671	ARG	4.1
1	E	682	GLN	4.0
1	E	667	GLU	3.7
1	E	575	ILE	3.7
1	E	669	GLN	3.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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(Å ²)	Q<0.9
2	LYZ	K	3	10/11	0.86	0.21	46,49,52,57	0
2	LYZ	L	3	10/11	0.92	0.19	41,43,53,53	0
2	LYZ	J	3	10/11	0.93	0.17	39,42,54,58	0
2	LYZ	I	3	10/11	0.94	0.21	29,35,48,53	0
2	LYZ	G	3	10/11	0.95	0.18	35,39,47,55	0
2	LYZ	H	3	10/11	0.95	0.13	30,40,51,52	0

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.