wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 – 07:16 am GMT

PDB ID	:	5A3F
Title	:	Crystal structure of the dynamin tetramer
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Deposited on	:	2015-05-29
Resolution	:	3.70 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:

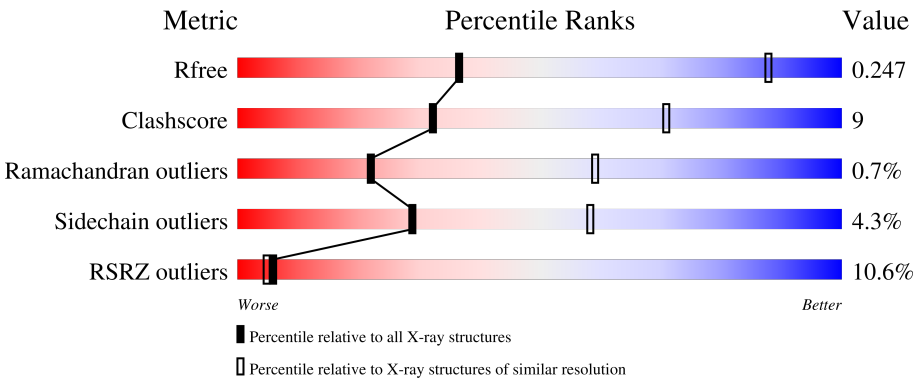
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 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	754	.% 66% 23% • 8%
1	B	754	15% 65% 9% 26%
1	C	754	2% 67% 23% • 7%
1	D	754	17% 64% 8% • 27%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18654 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 DYNAMIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	691	5548	3520	967	1035	26	0	0	0
1	B	555	3751	2325	688	724	14	0	0	0
1	C	700	5616	3557	983	1050	26	0	0	0
1	D	554	3739	2316	687	722	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

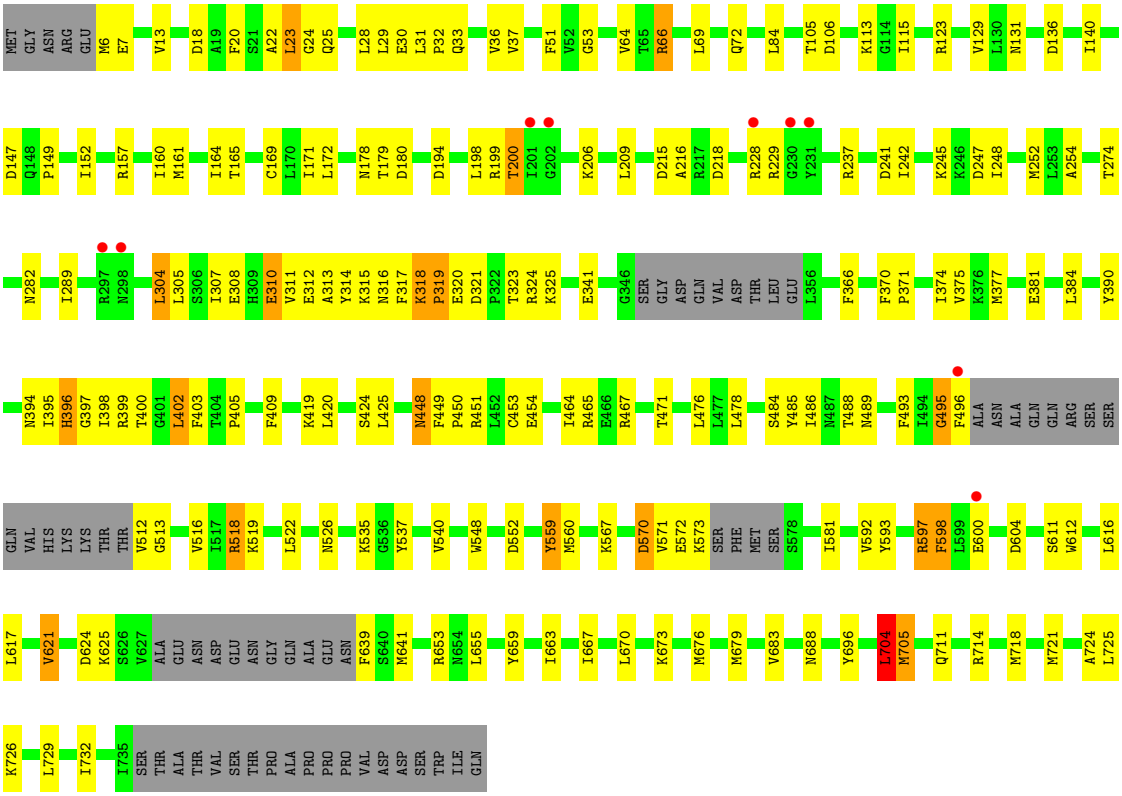
Chain	Residue	Modelled	Actual	Comment	Reference
A	361	SER	LYS	engineered mutation	UNP Q9UQ16
B	361	SER	LYS	engineered mutation	UNP Q9UQ16
C	361	SER	LYS	engineered mutation	UNP Q9UQ16
D	361	SER	LYS	engineered mutation	UNP Q9UQ16

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.

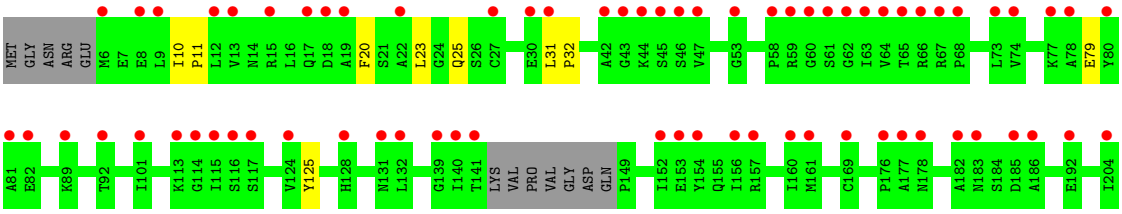
• Molecule 1: DYNAMIN 3

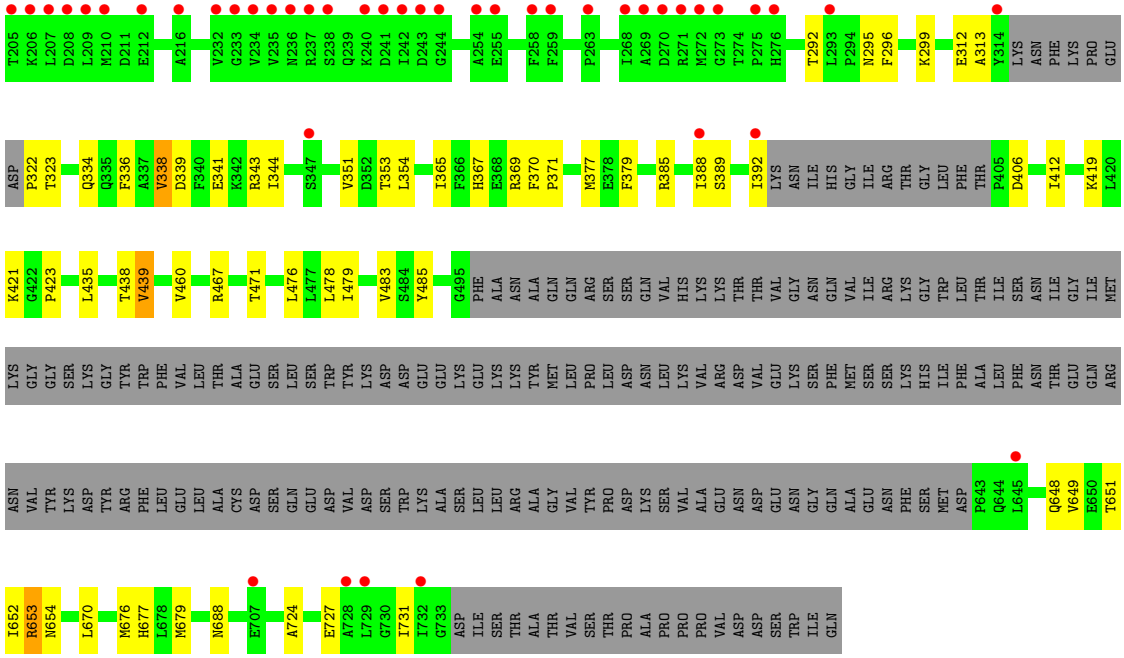
Chain A:



• Molecule 1: DYNAMIN 3

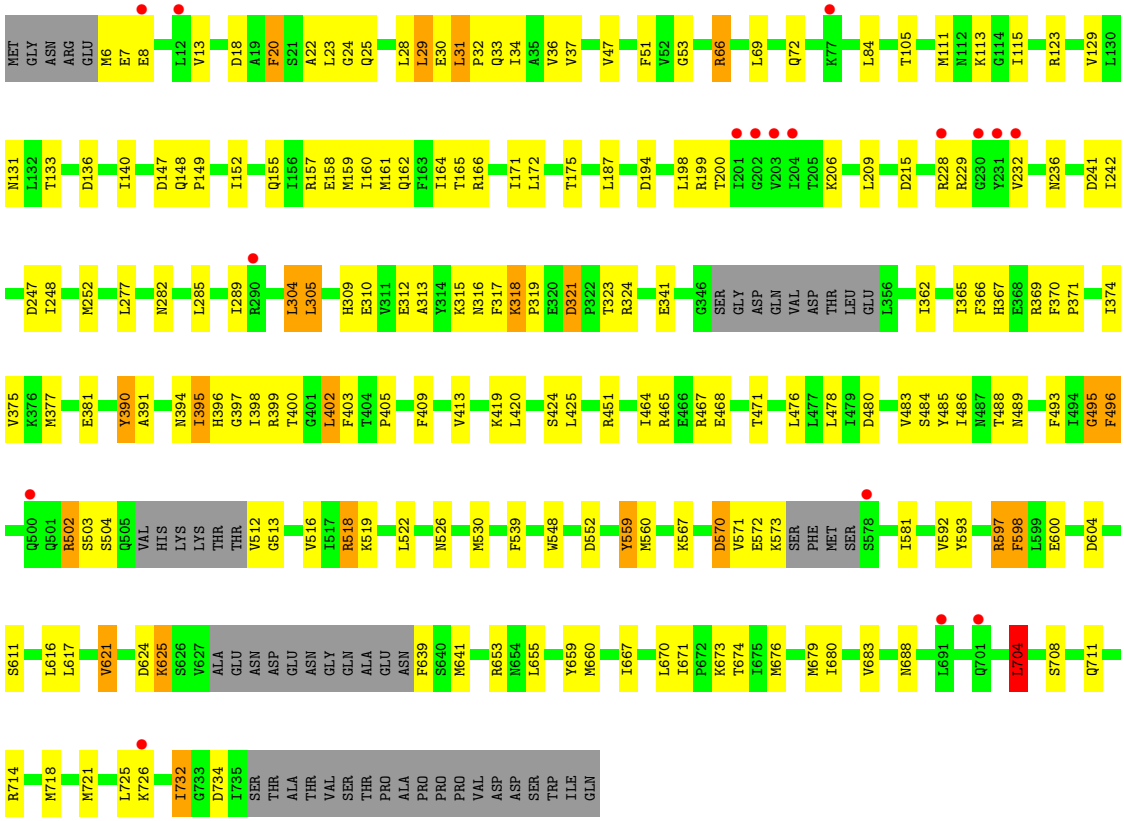
Chain B:





• Molecule 1: DYNAMIN 3

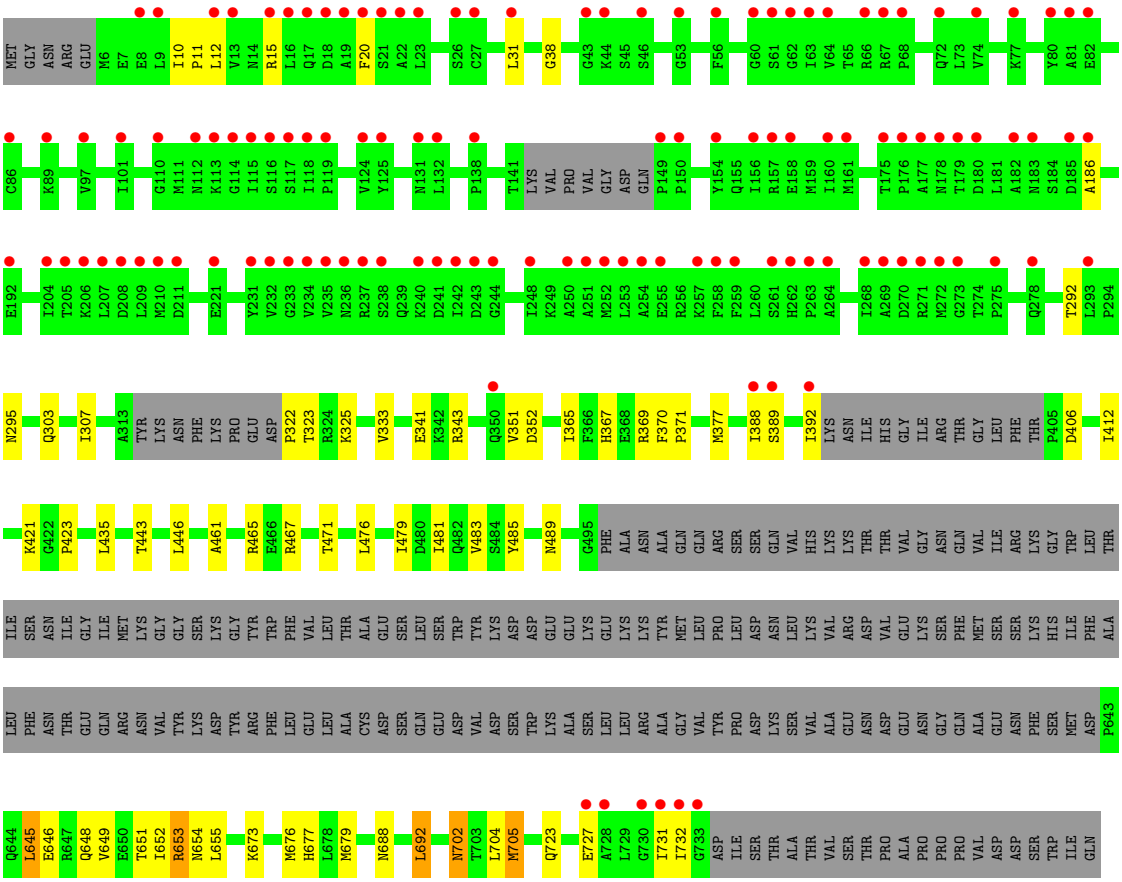
Chain C:



• Molecule 1: DYNAMIN 3

Chain D:

17%
64%
8%
27%


MET GLY ASN ARG GLU M6 E7 E8 L9 I10 P11 L12 V13 N14 R15 L16 Q17 D18 A19 F20 S21 A22 L23 S26 C27 L31 G38 G43 K44 S45 S46 G53 F56 G60 S61 G62 I63 V64 T65 R66 R67 P68 Q72 L73 V74 K77 Y80 A81 E82
C86 K89 V97 I101 G110 M111 N112 K113 G114 I115 S116 S117 I118 P119 V124 Y125 N131 L132 P138 T141 LYS VAL PRO VAL GLY ASP GLN P149 P150 Y154 Q155 I156 R157 E158 M159 I160 M161 T175 P176 A177 N178 T179 D180 L181 A182 N183 S184 D185 A186
E192 I204 T205 K206 L207 D208 L209 M210 D211 E221 Y231 V232 G233 V234 V235 N236 R237 S238 Q239 K240 D241 I242 D243 G244 I248 K249 A250 A251 M252 L253 A254 E255 R256 K257 F258 F259 L260 S261 H262 P263 A264 I268 A269 D270 R271 M272 G273 T274 P275 Q278 T292 L293 P294
N295 Q303 I307 A313 TYR LYS ASN PHE LYS PRO GLU ASP P322 T323 R324 K325 V333 E341 K342 R343 Q350 V351 D352 I365 F366 H367 E368 R369 F370 P371 M377 I388 S389 I392 LYS ASN ILE HIS GLY ILE ARG THR GLY LEU PHE THR P405 D406 I412
K421 G422 P423 L435 T443 L446 A461 R465 E466 R467 T471 L476 I479 D480 I481 Q482 V483 S484 Y485 N489 G495 PHE ALA ASN ALA GLN GLN ARG SER SER GLN VAL HIS LYS LYS THR THR VAL GLY ASN GLN VAL ILE ARG LYS GLY TRP LEU THR
ILE SER ASN ILE GLY ILE MET LYS GLY GLY SER LYS GLY TYR TRP PHE VAL LEU THR ALA GLU SER LEU SER TRP TYR LYS ASP ASP GLU GLU LYS GLU LYS LYS TYR MET LEU PRO LEU ASP ASN LEU LYS VAL ARG ASP VAL GLU LYS SER PHE MET SER SER LYS HIS ILE PHE ALA
LEU PHE ASN THR GLU GLN ARG ASN VAL TYR LYS ASP TYR ARG PHE LEU GLU LEU ALA CYS ASP SER GLN GLU ASP VAL ASP SER TRP LYS ALA SER LEU LEU ARG ALA GLY VAL TYR PRO ASP LYS SER VAL ALA GLU ASN ASP GLU ASN GLY GLN ALA GLU ASN PHE SER MET ASP P643
Q644 L645 E646 R647 Q648 V649 E650 T651 I652 R653 N654 L655 K673 M676 H677 L678 M679 N688 L692 N702 T703 L704 M705 Q723 E727 A728 L729 G730 I731 I732 G733 ASP ILE SER THR ALA THR VAL SER THR PRO ALA PRO PRO PRO VAL ASP ASP SER TRP ILE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.70Å 98.00Å 401.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.70 49.46 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.47-3.70) 98.8 (49.46-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.232 , 0.278 0.234 , 0.247	Depositor DCC
R_{free} test set	2472 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	142.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 134.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.368 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18654	wwPDB-VP
Average B, all atoms (Å^2)	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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	0.25	0/5635	0.47	2/7588 (0.0%)
1	B	0.25	0/3782	0.46	0/5134
1	C	0.25	0/5703	0.46	2/7679 (0.0%)
1	D	0.25	0/3769	0.46	0/5116
All	All	0.25	0/18889	0.46	4/25517 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	704	LEU	CA-CB-CG	6.24	129.65	115.30
1	C	495	GLY	N-CA-C	-6.00	98.10	113.10
1	A	495	GLY	N-CA-C	-5.39	99.62	113.10
1	C	704	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	LYS	Peptide
1	C	625	LYS	Peptide

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	5548	0	5670	120	0
1	B	3751	0	3183	43	0
1	C	5616	0	5733	132	0
1	D	3739	0	3174	43	0
All	All	18654	0	17760	322	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 9.

The worst 5 of 322 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:A:22:ALA:HB2	1:A:84:LEU:HD21	1.59	0.85
1:C:451:ARG:HD2	1:C:704:LEU:HA	1.64	0.80
1:A:23:LEU:O	1:A:25:GLN:N	2.16	0.77
1:C:6:MET:HG3	1:C:7:GLU:H	1.50	0.76
1:A:451:ARG:HD2	1:A:704:LEU:HA	1.68	0.74

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	681/754 (90%)	654 (96%)	21 (3%)	6 (1%)	17 54
1	B	545/754 (72%)	528 (97%)	15 (3%)	2 (0%)	34 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	690/754 (92%)	660 (96%)	22 (3%)	8 (1%)	13	48
1	D	544/754 (72%)	530 (97%)	13 (2%)	1 (0%)	47	78
All	All	2460/3016 (82%)	2372 (96%)	71 (3%)	17 (1%)	22	59

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	397	GLY
1	A	398	ILE
1	C	24	GLY
1	C	398	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	617/671 (92%)	588 (95%)	29 (5%)	26	56
1	B	293/671 (44%)	282 (96%)	11 (4%)	33	61
1	C	624/671 (93%)	595 (95%)	29 (5%)	27	57
1	D	292/671 (44%)	283 (97%)	9 (3%)	40	65
All	All	1826/2684 (68%)	1748 (96%)	78 (4%)	29	58

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	559	TYR
1	D	435	LEU
1	C	597	ARG
1	C	708	SER
1	D	692	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	691/754 (91%)	-0.28	9 (1%)	77	67	86, 200, 339, 530	0
1	B	555/754 (73%)	1.07	113 (20%)	1	0	92, 227, 356, 545	253 (45%)
1	C	700/754 (92%)	-0.25	17 (2%)	59	47	87, 201, 333, 458	0
1	D	554/754 (73%)	1.13	127 (22%)	0	0	93, 225, 352, 464	253 (45%)
All	All	2500/3016 (82%)	0.34	266 (10%)	6	5	86, 211, 346, 545	506 (20%)

The worst 5 of 266 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	241	ASP	22.7
1	D	116	SER	22.3
1	B	60	GLY	21.7
1	B	61	SER	16.3
1	D	233	GLY	15.9

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.