



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:26 PM GMT

PDB ID : 4RWT
Title : Structure of actin-Lmod complex
Authors : Chen, X.; Ni, F.; Wang, Q.
Deposited on : 2014-12-05
Resolution : 2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

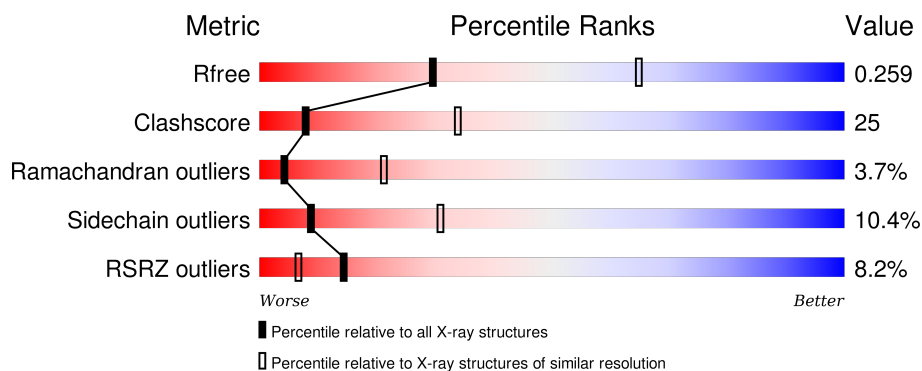
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	384	
1	B	384	
2	C	506	
2	D	506	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9317 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 Actin-5C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2873	1817	485	550	21			
1	B	369	Total	C	N	O	S	0	0	0
			2871	1815	485	550	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLU	LYS	ENGINEERED MUTATION	UNP P10987
A	322	LYS	PRO	ENGINEERED MUTATION	UNP P10987
A	376	ALA	-	EXPRESSION TAG	UNP P10987
A	377	SER	-	EXPRESSION TAG	UNP P10987
A	378	HIS	-	EXPRESSION TAG	UNP P10987
A	379	HIS	-	EXPRESSION TAG	UNP P10987
A	380	HIS	-	EXPRESSION TAG	UNP P10987
A	381	HIS	-	EXPRESSION TAG	UNP P10987
A	382	HIS	-	EXPRESSION TAG	UNP P10987
A	383	HIS	-	EXPRESSION TAG	UNP P10987
B	291	GLU	LYS	ENGINEERED MUTATION	UNP P10987
B	322	LYS	PRO	ENGINEERED MUTATION	UNP P10987
B	376	ALA	-	EXPRESSION TAG	UNP P10987
B	377	SER	-	EXPRESSION TAG	UNP P10987
B	378	HIS	-	EXPRESSION TAG	UNP P10987
B	379	HIS	-	EXPRESSION TAG	UNP P10987
B	380	HIS	-	EXPRESSION TAG	UNP P10987
B	381	HIS	-	EXPRESSION TAG	UNP P10987
B	382	HIS	-	EXPRESSION TAG	UNP P10987
B	383	HIS	-	EXPRESSION TAG	UNP P10987

- Molecule 2 is a protein called Leiomodin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	168	Total 1338	C 829	N 242	O 259	S 8	0	0	0
2	D	280	Total 2171	C 1340	N 398	O 423	S 10	0	0	0

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	EXPRESSION TAG	UNP Q6P5Q4
C	-9	ALA	-	EXPRESSION TAG	UNP Q6P5Q4
C	-8	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-7	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-6	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-5	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-4	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-3	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-2	VAL	-	EXPRESSION TAG	UNP Q6P5Q4
C	-1	GLY	-	EXPRESSION TAG	UNP Q6P5Q4
C	0	THR	-	EXPRESSION TAG	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	LEU	DELETION	UNP Q6P5Q4
C	?	-	ILE	DELETION	UNP Q6P5Q4
C	?	-	PHE	DELETION	UNP Q6P5Q4
C	?	-	THR	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	ASN	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	VAL	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	VAL	DELETION	UNP Q6P5Q4
C	?	-	TYR	DELETION	UNP Q6P5Q4
C	?	-	THR	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLN	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLN	DELETION	UNP Q6P5Q4
C	?	-	ARG	DELETION	UNP Q6P5Q4
C	?	-	LEU	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	426	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	427	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	428	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	429	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	431	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	432	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	434	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	435	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	-10	MET	-	EXPRESSION TAG	UNP Q6P5Q4
D	-9	ALA	-	EXPRESSION TAG	UNP Q6P5Q4
D	-8	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-7	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-6	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-5	HIS	-	EXPRESSION TAG	UNP Q6P5Q4



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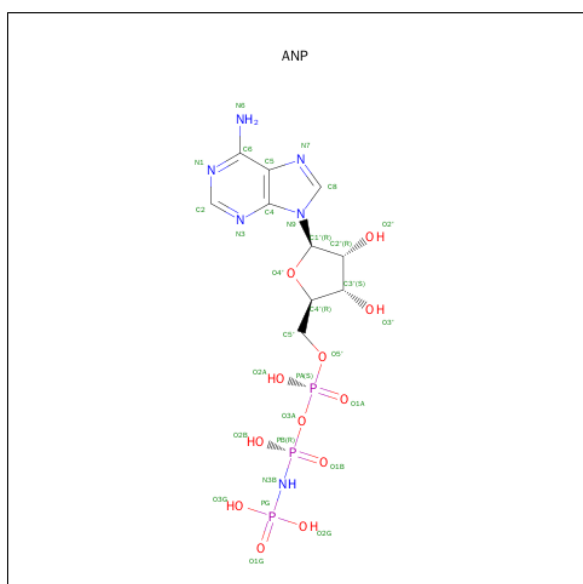
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-3	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-2	VAL	-	EXPRESSION TAG	UNP Q6P5Q4
D	-1	GLY	-	EXPRESSION TAG	UNP Q6P5Q4
D	0	THR	-	EXPRESSION TAG	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	LEU	DELETION	UNP Q6P5Q4
D	?	-	ILE	DELETION	UNP Q6P5Q4
D	?	-	PHE	DELETION	UNP Q6P5Q4
D	?	-	THR	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	ASN	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	VAL	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	VAL	DELETION	UNP Q6P5Q4
D	?	-	TYR	DELETION	UNP Q6P5Q4
D	?	-	THR	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLN	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLN	DELETION	UNP Q6P5Q4
D	?	-	ARG	DELETION	UNP Q6P5Q4
D	?	-	LEU	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	426	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	427	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	428	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	429	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	431	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	432	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	434	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	435	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

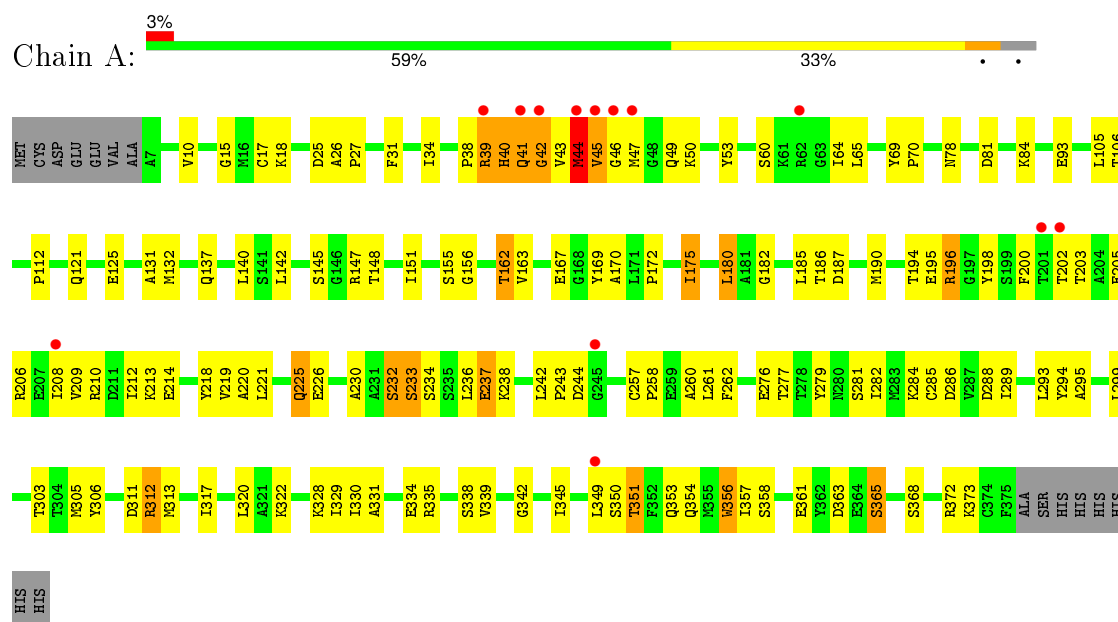
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

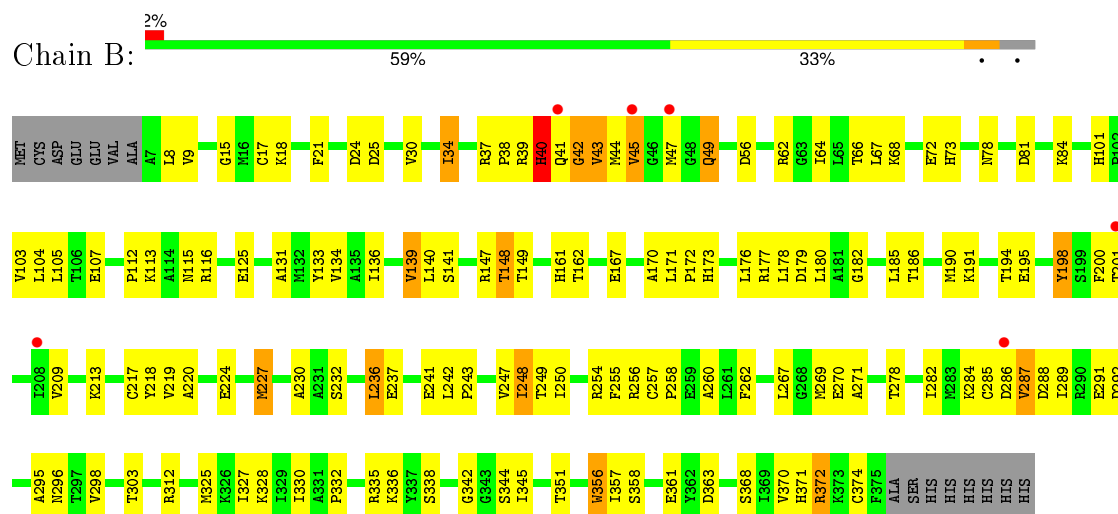
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

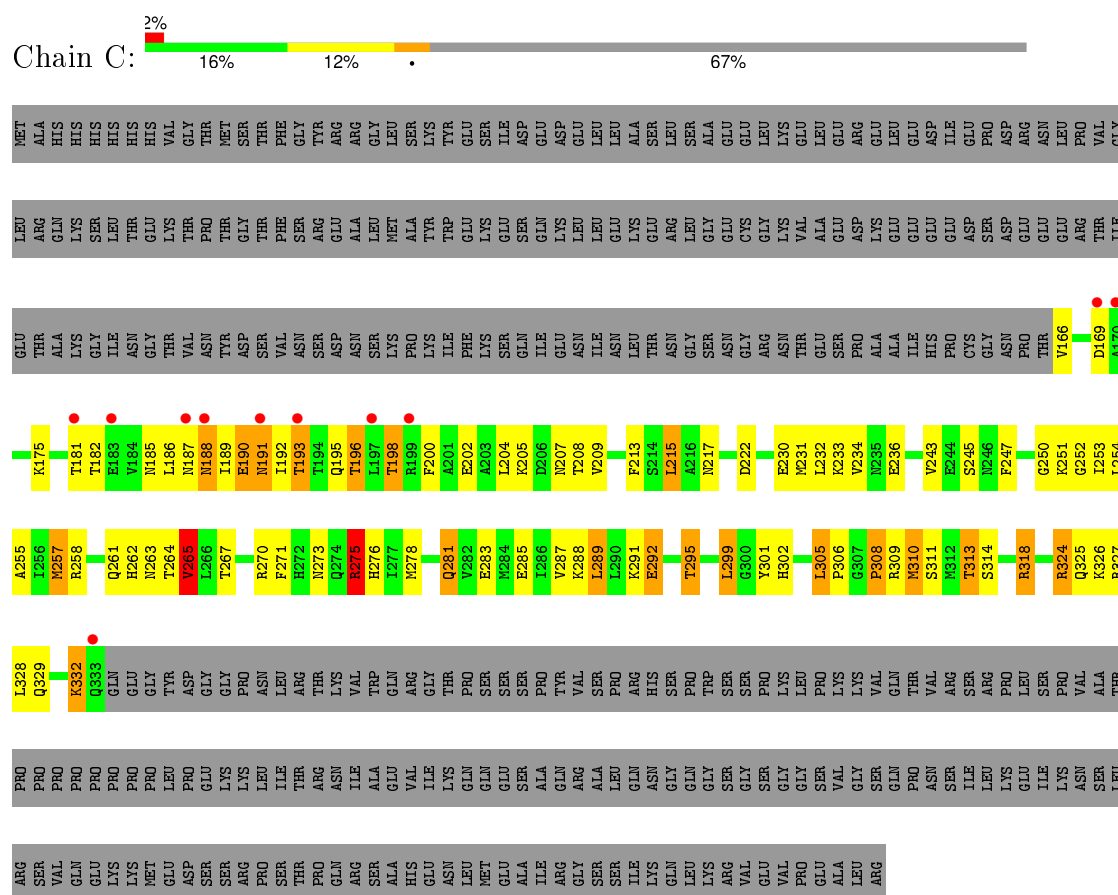
• Molecule 1: Actin-5C



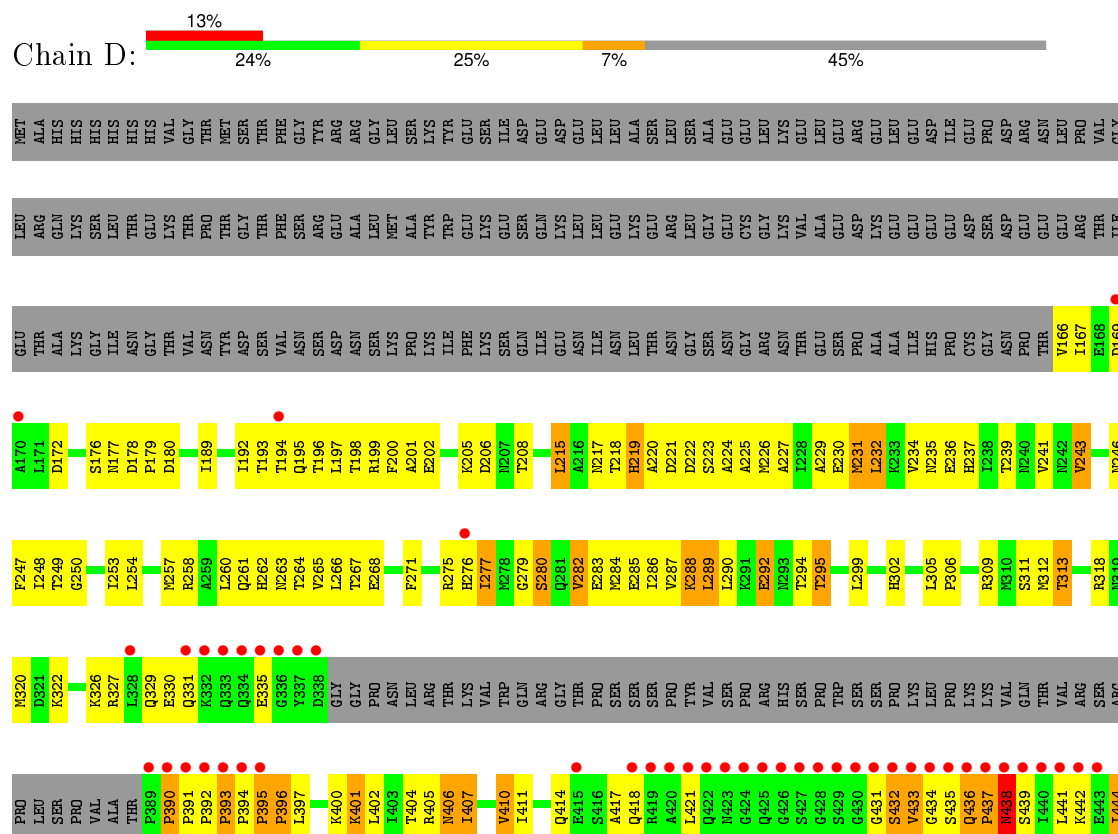
• Molecule 1: Actin-5C

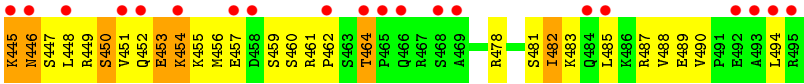


• Molecule 2: Leiomodrin-2



- Molecule 2: Leiomodrin-2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.35Å 65.65Å 81.92Å 101.29° 90.94° 107.97°	Depositor
Resolution (Å)	51.07 – 2.98 47.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (51.07-2.98) 90.5 (47.15-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.257 0.249 , 0.259	Depositor DCC
R_{free} test set	1288 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 25186 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9317	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	0.47	0/2934	0.63	1/3973 (0.0%)
1	B	0.49	0/2932	0.63	0/3970
2	C	0.46	1/1352 (0.1%)	0.57	0/1823
2	D	0.61	0/2199	0.64	0/2966
All	All	0.51	1/9417 (0.0%)	0.62	1/12732 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	332	LYS	CE-NZ	5.20	1.62	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	MET	N-CA-C	5.07	124.69	111.00

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	2873	0	2842	123	2
1	B	2871	0	2834	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1338	0	1364	89	0
2	D	2171	0	2190	204	2
3	A	31	0	13	2	0
3	B	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9317	0	9256	462	2

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 25.

All (462) 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:44:MET:O	1:A:46:GLY:N	1.76	1.19
1:A:121:GLN:NE2	2:D:320:MET:HB3	1.59	1.18
2:D:390:PRO:HB2	2:D:391:PRO:CD	1.77	1.14
2:C:187:ASN:HD22	1:B:49:GLN:HA	0.93	1.08
2:C:193:THR:HB	2:C:196:THR:HB	1.11	1.07
2:C:187:ASN:ND2	1:B:49:GLN:HA	1.70	1.06
1:A:125:GLU:OE2	2:D:327:ARG:NH2	1.91	1.01
2:C:310:MET:HB3	2:D:448:LEU:HB2	1.37	1.01
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.18	1.01
1:A:44:MET:O	1:A:45:VAL:C	2.00	0.99
2:D:448:LEU:HD21	2:D:452:GLN:HB2	1.43	0.99
1:A:351:THR:HB	2:D:411:ILE:CG2	1.93	0.99
2:C:187:ASN:HD22	1:B:49:GLN:CA	1.76	0.98
1:A:345:ILE:HG22	2:D:402:LEU:HD13	1.43	0.97
2:D:390:PRO:HB2	2:D:391:PRO:HD3	1.46	0.96
1:B:44:MET:HB3	1:B:64:ILE:HD12	1.46	0.96
1:A:60:SER:HB2	2:D:390:PRO:HD2	1.46	0.95
1:A:38:PRO:HB3	1:A:43:VAL:HG11	1.44	0.95
1:B:43:VAL:O	1:B:43:VAL:HG23	1.64	0.95
2:D:435:SER:HA	1:B:270:GLU:HG2	1.46	0.95
2:D:434:GLY:HA2	1:B:271:ALA:HB2	1.49	0.94
2:D:435:SER:C	2:D:437:PRO:HD3	1.90	0.92
1:B:39:ARG:O	1:B:40:HIS:HB2	1.70	0.91
1:A:121:GLN:HE22	2:D:320:MET:HB3	1.20	0.91
2:D:257:MET:HE1	2:D:290:LEU:HD11	1.54	0.90
2:C:311:SER:OG	2:D:452:GLN:HG3	1.74	0.87
2:C:193:THR:CB	2:C:196:THR:HB	2.02	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:THR:O	2:D:220:ALA:N	2.07	0.86
1:A:351:THR:HB	2:D:411:ILE:HG21	1.58	0.86
2:D:261:GLN:NE2	2:D:292:GLU:OE1	2.09	0.85
2:D:433:VAL:O	1:B:270:GLU:HG3	1.76	0.84
2:C:310:MET:HG2	2:D:448:LEU:H	1.42	0.84
2:C:309:ARG:O	2:C:313:THR:HG22	1.77	0.84
2:D:250:GLY:HA3	2:D:282:VAL:HG11	1.59	0.84
2:D:257:MET:HE1	2:D:290:LEU:CD1	2.11	0.80
2:C:202:GLU:HA	2:C:205:LYS:HB2	1.63	0.80
2:C:192:ILE:O	2:C:193:THR:OG1	1.99	0.80
2:D:264:THR:HA	2:D:295:THR:HG21	1.65	0.79
2:D:243:VAL:CG1	2:D:243:VAL:O	2.31	0.79
2:D:294:THR:CG2	2:D:322:LYS:HD2	2.14	0.78
1:B:191:LYS:O	1:B:195:GLU:HG2	1.84	0.78
2:D:457:GLU:HB2	1:B:371:HIS:CD2	2.18	0.78
1:A:196:ARG:CG	1:A:196:ARG:HH11	1.97	0.77
2:D:390:PRO:HB2	2:D:391:PRO:HD2	1.64	0.77
2:D:232:LEU:HD11	2:D:266:LEU:HD22	1.67	0.77
1:A:351:THR:HB	2:D:411:ILE:HG22	1.67	0.77
2:D:457:GLU:HB3	1:B:113:LYS:HD3	1.64	0.77
2:D:457:GLU:H	1:B:113:LYS:HZ2	1.34	0.76
2:C:189:ILE:HG13	2:C:191:ASN:HB2	1.68	0.75
2:D:435:SER:HA	1:B:270:GLU:CG	2.17	0.75
2:D:457:GLU:HG2	1:B:113:LYS:NZ	2.03	0.74
1:A:121:GLN:NE2	2:D:320:MET:CB	2.47	0.74
2:D:405:ARG:HG2	2:D:406:ASN:H	1.52	0.73
2:C:271:PHE:HE2	2:C:299:LEU:HD21	1.54	0.73
1:B:39:ARG:O	1:B:40:HIS:CB	2.37	0.73
2:D:451:VAL:HG12	2:D:452:GLN:H	1.55	0.72
1:B:248:ILE:HG12	1:B:249:THR:N	2.05	0.72
2:D:277:ILE:HG12	2:D:279:GLY:H	1.55	0.72
2:D:294:THR:HG23	2:D:322:LYS:HD2	1.72	0.72
2:D:167:ILE:HD11	2:D:189:ILE:HG21	1.72	0.72
2:C:328:LEU:O	2:C:332:LYS:HB2	1.90	0.71
2:D:166:VAL:HG12	2:D:167:ILE:H	1.55	0.71
2:D:485:LEU:HD11	1:B:345:ILE:HG13	1.71	0.71
1:A:64:ILE:O	1:A:64:ILE:HG22	1.91	0.71
1:A:60:SER:O	2:D:390:PRO:CG	2.38	0.71
1:A:39:ARG:HG3	1:A:64:ILE:C	2.11	0.70
2:D:459:SER:HB3	1:B:372:ARG:HE	1.56	0.70
1:B:39:ARG:N	1:B:64:ILE:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:LYS:O	2:C:329:GLN:HG2	1.90	0.70
1:A:351:THR:CG2	2:D:411:ILE:HG22	2.22	0.70
2:D:435:SER:CA	1:B:270:GLU:HG2	2.19	0.70
1:A:284:LYS:HB2	1:A:284:LYS:NZ	2.06	0.69
2:D:234:VAL:O	2:D:234:VAL:HG12	1.92	0.69
2:D:393:PRO:O	2:D:395:PRO:HD3	1.93	0.69
1:B:43:VAL:CG2	1:B:43:VAL:O	2.35	0.69
2:C:193:THR:HB	2:C:196:THR:CB	2.06	0.69
1:A:196:ARG:NH1	1:A:196:ARG:HG2	1.99	0.69
2:D:309:ARG:O	2:D:313:THR:HG22	1.92	0.69
2:C:251:LYS:N	2:C:251:LYS:HD2	2.08	0.69
1:A:221:LEU:HD21	1:A:311:ASP:HB2	1.73	0.69
1:A:349:LEU:HD11	2:D:407:ILE:HG23	1.75	0.68
1:A:148:THR:OG1	2:D:410:VAL:HG21	1.92	0.68
1:A:40:HIS:O	1:A:41:GLN:HB2	1.94	0.68
2:C:187:ASN:O	2:C:189:ILE:N	2.26	0.68
1:B:43:VAL:O	1:B:45:VAL:N	2.27	0.68
1:B:64:ILE:O	1:B:64:ILE:HG12	1.92	0.68
2:D:253:ILE:O	2:D:257:MET:HG2	1.94	0.68
1:A:205:GLU:O	1:A:208:ILE:HG13	1.92	0.68
2:D:236:GLU:HA	2:D:265:VAL:HG21	1.73	0.68
1:A:39:ARG:N	1:A:64:ILE:O	2.27	0.68
2:D:438:ASN:O	2:D:442:LYS:HG2	1.94	0.67
1:B:180:LEU:HD13	1:B:267:LEU:HD12	1.77	0.67
1:A:10:VAL:HB	1:A:105:LEU:CD2	2.25	0.67
2:D:390:PRO:CB	2:D:391:PRO:HD3	2.23	0.67
2:C:324:ARG:HA	2:C:327:ARG:NH1	2.10	0.67
1:B:370:VAL:O	1:B:374:CYS:HB2	1.94	0.67
2:C:275:ARG:HG3	2:C:276:HIS:H	1.60	0.67
1:A:180:LEU:HD21	1:A:261:LEU:HD23	1.77	0.66
2:C:230:GLU:HG3	2:C:233:LYS:HE3	1.78	0.66
2:D:390:PRO:CB	2:D:391:PRO:CD	2.63	0.66
2:D:435:SER:CB	2:D:437:PRO:HD3	2.26	0.65
2:D:267:THR:HG23	2:D:268:GLU:HG3	1.78	0.65
1:A:163:VAL:HG13	1:A:175:ILE:CD1	2.26	0.65
2:C:196:THR:O	2:C:200:PHE:HD1	1.77	0.65
1:A:121:GLN:HE21	2:D:320:MET:HB3	1.56	0.65
2:D:215:LEU:HD11	2:D:243:VAL:HG22	1.78	0.65
1:A:148:THR:HG21	1:A:167:GLU:OE2	1.97	0.65
1:B:171:LEU:HB3	1:B:173:HIS:CE1	2.31	0.65
2:D:257:MET:CE	2:D:290:LEU:HG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:HB2	2:D:390:PRO:CD	2.26	0.64
1:B:39:ARG:HB2	1:B:64:ILE:O	1.96	0.64
2:C:257:MET:HB3	2:C:289:LEU:HD13	1.77	0.64
1:A:220:ALA:O	1:A:312:ARG:HD2	1.98	0.64
2:D:457:GLU:HG2	1:B:113:LYS:HZ2	1.62	0.64
1:A:306:TYR:CE2	3:A:401:ANP:H2	2.32	0.64
1:A:219:VAL:HG11	1:A:262:PHE:CE1	2.32	0.64
2:D:431:GLY:HA3	1:B:176:LEU:HD22	1.80	0.64
1:A:276:GLU:HG2	1:A:320:LEU:HD11	1.79	0.64
1:B:250:ILE:HD12	1:B:254:ARG:HG2	1.80	0.64
2:D:241:VAL:HG23	2:D:266:LEU:HD11	1.79	0.63
2:D:459:SER:HB3	1:B:372:ARG:NE	2.12	0.63
2:D:437:PRO:O	2:D:441:LEU:HG	1.99	0.63
1:A:64:ILE:O	1:A:64:ILE:CG2	2.46	0.63
2:D:243:VAL:HG12	2:D:243:VAL:O	1.97	0.63
1:A:351:THR:CB	2:D:411:ILE:HG22	2.28	0.63
2:D:439:SER:O	2:D:445:LYS:NZ	2.31	0.63
2:D:432:SER:O	2:D:434:GLY:N	2.29	0.63
2:D:457:GLU:CB	1:B:371:HIS:CD2	2.82	0.63
1:A:25:ASP:HB2	2:D:401:LYS:H	1.64	0.63
1:B:220:ALA:O	1:B:312:ARG:HD3	1.98	0.63
2:C:278:MET:CE	2:C:278:MET:HA	2.29	0.63
1:A:218:TYR:OH	1:A:226:GLU:OE1	2.15	0.63
1:A:242:LEU:HB3	1:A:243:PRO:HD2	1.80	0.63
1:B:191:LYS:O	1:B:195:GLU:CG	2.46	0.62
1:B:219:VAL:HG11	1:B:262:PHE:CE1	2.33	0.62
2:C:302:HIS:HB2	1:B:78:ASN:HD22	1.63	0.62
2:C:327:ARG:NH2	1:B:363:ASP:OD1	2.33	0.62
2:C:291:LYS:O	2:C:318:ARG:NH2	2.28	0.62
1:B:44:MET:HE3	1:B:64:ILE:HB	1.82	0.61
2:C:258:ARG:HG3	2:C:289:LEU:HD21	1.83	0.61
2:C:243:VAL:O	2:C:271:PHE:HA	2.00	0.61
2:D:275:ARG:HG3	2:D:276:HIS:H	1.64	0.61
2:D:219:HIS:O	2:D:219:HIS:ND1	2.34	0.61
2:C:217:ASN:OD1	1:B:43:VAL:HG12	2.00	0.61
2:C:310:MET:CE	1:B:115:ASN:OD1	2.49	0.61
2:D:457:GLU:HB2	1:B:371:HIS:HD2	1.66	0.61
2:C:193:THR:CG2	2:C:196:THR:H	2.13	0.61
1:B:284:LYS:HB2	1:B:284:LYS:NZ	2.15	0.60
2:C:287:VAL:HG11	2:C:311:SER:HB2	1.84	0.60
1:A:286:ASP:HA	1:B:195:GLU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:HG21	1:A:277:THR:O	2.01	0.60
2:D:454:LYS:H	2:D:454:LYS:HD3	1.65	0.60
2:D:239:THR:HB	2:D:267:THR:HG22	1.83	0.60
2:C:287:VAL:HG11	2:C:311:SER:CB	2.31	0.60
2:C:236:GLU:HA	2:C:265:VAL:HG21	1.83	0.60
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.84	0.60
1:A:363:ASP:OD1	2:D:327:ARG:NH1	2.20	0.59
1:A:156:GLY:HA2	3:A:401:ANP:O1A	2.02	0.59
2:C:325:GLN:O	2:C:328:LEU:HB3	2.01	0.59
1:A:43:VAL:HG13	1:A:64:ILE:HG21	1.85	0.59
2:D:434:GLY:CA	1:B:271:ALA:HB2	2.29	0.59
2:D:464:THR:O	2:D:464:THR:HG22	2.02	0.59
2:D:451:VAL:HG12	2:D:452:GLN:N	2.17	0.59
2:D:435:SER:HB3	2:D:437:PRO:HD3	1.85	0.59
1:B:230:ALA:HB2	1:B:236:LEU:HD23	1.85	0.59
2:C:310:MET:CB	2:D:448:LEU:HB2	2.25	0.58
2:D:222:ASP:OD1	2:D:249:THR:OG1	2.19	0.58
2:D:258:ARG:O	2:D:261:GLN:HB2	2.03	0.58
1:A:78:ASN:ND2	2:D:302:HIS:HB2	2.18	0.58
2:D:410:VAL:O	2:D:414:GLN:N	2.37	0.57
1:B:147:ARG:NH2	1:B:330:ILE:HG12	2.19	0.57
2:D:258:ARG:HG3	2:D:289:LEU:HD21	1.87	0.57
2:D:194:THR:CG2	2:D:223:SER:OG	2.53	0.57
2:C:193:THR:HG22	2:C:196:THR:H	1.70	0.57
2:C:285:GLU:O	2:C:289:LEU:HB2	2.05	0.57
1:B:104:LEU:HD12	1:B:133:TYR:HB3	1.87	0.56
1:A:284:LYS:HB2	1:A:284:LYS:HZ2	1.69	0.56
2:D:405:ARG:HG2	2:D:406:ASN:N	2.18	0.56
1:A:163:VAL:HG13	1:A:175:ILE:HD11	1.87	0.56
1:B:136:ILE:HB	1:B:139:VAL:HG13	1.86	0.56
1:A:151:ILE:HD11	1:A:162:THR:OG1	2.06	0.56
2:C:306:PRO:HB2	2:D:446:ASN:O	2.05	0.56
2:D:407:ILE:HD13	2:D:407:ILE:O	2.06	0.55
1:B:161:HIS:CE1	1:B:177:ARG:HG3	2.40	0.55
2:D:449:ARG:O	2:D:451:VAL:N	2.39	0.55
2:C:305:LEU:HB3	2:C:308:PRO:HG2	1.88	0.55
1:A:125:GLU:CD	2:D:327:ARG:HH21	2.06	0.55
2:D:457:GLU:CG	1:B:113:LYS:NZ	2.70	0.55
1:B:358:SER:HB2	1:B:361:GLU:HG3	1.88	0.55
2:D:294:THR:HG23	2:D:322:LYS:NZ	2.22	0.55
1:B:41:GLN:O	1:B:43:VAL:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:GLN:NE2	2:C:292:GLU:OE2	2.39	0.55
2:D:193:THR:HB	2:D:196:THR:H	1.71	0.55
1:A:230:ALA:HB2	1:A:236:LEU:HD12	1.89	0.55
2:D:431:GLY:CA	1:B:176:LEU:HD22	2.37	0.54
1:B:136:ILE:HB	1:B:139:VAL:CG1	2.38	0.54
1:B:296:ASN:O	1:B:298:VAL:HG23	2.07	0.54
1:B:186:THR:OG1	1:B:213:LYS:NZ	2.35	0.54
2:D:327:ARG:O	2:D:331:GLN:HB3	2.07	0.54
2:D:258:ARG:HG3	2:D:289:LEU:HD11	1.90	0.54
2:D:166:VAL:N	2:D:169:ASP:OD2	2.40	0.54
2:D:444:ILE:HG13	2:D:445:LYS:N	2.23	0.54
1:A:25:ASP:HB2	2:D:400:LYS:H	1.72	0.54
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.89	0.54
2:C:245:SER:HA	2:C:273:ASN:O	2.08	0.54
1:A:299:LEU:HD12	1:A:331:ALA:HB2	1.89	0.54
2:D:431:GLY:O	2:D:432:SER:C	2.47	0.54
2:C:251:LYS:N	2:C:251:LYS:CD	2.71	0.54
1:A:353:GLN:O	1:A:356:TRP:HD1	1.91	0.54
2:D:400:LYS:O	2:D:401:LYS:HB2	2.08	0.53
1:B:177:ARG:NH1	1:B:179:ASP:OD1	2.41	0.53
2:C:263:ASN:C	2:C:263:ASN:OD1	2.46	0.53
1:B:198:TYR:HB2	1:B:200:PHE:CE1	2.44	0.53
2:D:243:VAL:HG13	2:D:243:VAL:O	2.06	0.53
1:A:187:ASP:OD1	1:A:206:ARG:NH2	2.36	0.53
2:D:299:LEU:HD22	2:D:312:MET:CE	2.38	0.53
1:A:358:SER:HB2	1:A:361:GLU:HG3	1.91	0.53
1:A:142:LEU:O	1:A:145:SER:OG	2.25	0.53
1:A:60:SER:O	2:D:390:PRO:HG3	2.09	0.53
1:A:163:VAL:HG13	1:A:175:ILE:HD13	1.90	0.53
1:B:227:MET:CE	1:B:256:ARG:HD2	2.38	0.53
2:D:294:THR:HG23	2:D:322:LYS:HZ2	1.73	0.53
2:D:455:LYS:HE3	1:B:112:PRO:HB3	1.91	0.53
2:D:457:GLU:OE1	1:B:371:HIS:CG	2.62	0.53
1:A:10:VAL:HB	1:A:105:LEU:HD23	1.90	0.52
2:C:310:MET:HE1	1:B:115:ASN:OD1	2.08	0.52
2:D:239:THR:O	2:D:267:THR:HG22	2.09	0.52
1:B:37:ARG:NH2	1:B:81:ASP:OD2	2.43	0.52
1:A:335:ARG:HA	1:A:338:SER:HB3	1.92	0.52
1:B:198:TYR:CD2	1:B:198:TYR:N	2.71	0.52
1:A:190:MET:HG3	1:A:209:VAL:HG11	1.91	0.52
2:D:478:ARG:HG3	1:B:148:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:490:VAL:HG21	1:B:30:VAL:CG2	2.40	0.52
2:D:294:THR:HG22	2:D:294:THR:O	2.10	0.52
1:A:47:MET:HE2	1:A:53:TYR:HE1	1.74	0.52
2:D:202:GLU:HA	2:D:205:LYS:HB2	1.91	0.52
2:D:435:SER:C	2:D:437:PRO:CD	2.73	0.52
1:B:131:ALA:HA	1:B:357:ILE:O	2.10	0.52
1:A:163:VAL:HG22	1:A:175:ILE:HD13	1.91	0.52
2:C:217:ASN:CG	1:B:43:VAL:HG12	2.30	0.52
1:B:241:GLU:HG2	1:B:247:VAL:HG22	1.90	0.52
2:D:243:VAL:HG13	2:D:248:ILE:HD12	1.92	0.51
1:A:221:LEU:HD21	1:A:311:ASP:CB	2.41	0.51
2:C:234:VAL:HG12	2:C:234:VAL:O	2.10	0.51
1:A:237:GLU:HG2	1:A:238:LYS:N	2.25	0.51
1:B:149:THR:OG1	1:B:167:GLU:OE2	2.23	0.51
2:C:188:ASN:HA	2:C:217:ASN:HB3	1.93	0.51
1:B:39:ARG:HB2	1:B:64:ILE:C	2.31	0.51
1:B:198:TYR:CE2	1:B:248:ILE:HD12	2.45	0.51
1:A:47:MET:CE	1:A:53:TYR:CE1	2.93	0.51
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.93	0.51
1:B:103:VAL:HG12	1:B:105:LEU:CD1	2.40	0.51
1:B:180:LEU:HD13	1:B:267:LEU:CD1	2.40	0.51
1:A:194:THR:HA	1:A:198:TYR:O	2.11	0.51
1:B:9:VAL:HG21	1:B:344:SER:HA	1.93	0.51
2:D:257:MET:CE	2:D:290:LEU:CG	2.89	0.51
1:A:43:VAL:HB	2:D:217:ASN:HD21	1.76	0.51
2:D:455:LYS:HD2	1:B:113:LYS:HB2	1.91	0.51
1:A:106:THR:HB	1:A:137:GLN:HG3	1.92	0.51
2:C:306:PRO:CB	2:D:446:ASN:O	2.59	0.50
2:D:454:LYS:CD	2:D:454:LYS:H	2.24	0.50
2:D:299:LEU:HD22	2:D:312:MET:HE1	1.93	0.50
2:D:331:GLN:HA	2:D:335:GLU:OE1	2.11	0.50
2:D:435:SER:OG	1:B:269:MET:HA	2.10	0.50
1:B:194:THR:HA	1:B:198:TYR:O	2.12	0.50
1:B:107:GLU:OE1	1:B:116:ARG:HG2	2.11	0.50
1:A:233:SER:OG	1:A:234:SER:N	2.45	0.50
2:D:435:SER:HA	1:B:270:GLU:CD	2.32	0.50
2:D:457:GLU:HG2	1:B:113:LYS:HZ3	1.75	0.50
1:B:131:ALA:HB1	1:B:356:TRP:HB3	1.94	0.50
2:C:243:VAL:HG23	2:C:243:VAL:O	2.12	0.50
1:A:372:ARG:HH12	1:A:373:LYS:HG2	1.77	0.50
1:A:317:ILE:O	1:A:317:ILE:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ARG:HA	1:B:338:SER:HB3	1.92	0.50
2:D:451:VAL:CG1	2:D:452:GLN:H	2.24	0.50
2:D:257:MET:HE3	2:D:290:LEU:HG	1.93	0.50
1:B:242:LEU:HB3	1:B:243:PRO:HD2	1.93	0.50
2:D:229:ALA:O	2:D:232:LEU:HB2	2.12	0.50
2:C:188:ASN:OD1	2:C:217:ASN:ND2	2.45	0.49
1:B:64:ILE:CG1	1:B:64:ILE:O	2.61	0.49
1:A:60:SER:O	2:D:390:PRO:HG2	2.10	0.49
2:D:194:THR:HG23	2:D:223:SER:OG	2.10	0.49
1:B:170:ALA:O	1:B:172:PRO:HD3	2.13	0.49
2:D:258:ARG:CG	2:D:289:LEU:HD21	2.43	0.49
1:A:78:ASN:HD22	2:D:302:HIS:HB2	1.77	0.49
1:A:131:ALA:HA	1:A:357:ILE:O	2.11	0.49
1:B:248:ILE:CG1	1:B:249:THR:N	2.74	0.49
2:C:258:ARG:CG	2:C:289:LEU:HD21	2.42	0.49
2:C:314:SER:HB3	2:D:453:GLU:OE1	2.13	0.49
2:D:447:SER:OG	1:B:112:PRO:HG3	2.13	0.49
1:A:41:GLN:O	1:A:43:VAL:N	2.45	0.48
1:A:43:VAL:O	1:A:44:MET:C	2.50	0.48
1:B:37:ARG:HB3	1:B:38:PRO:HD2	1.95	0.48
1:A:170:ALA:O	1:A:172:PRO:HD3	2.12	0.48
2:C:185:ASN:OD1	2:C:187:ASN:HB3	2.12	0.48
2:D:457:GLU:CD	1:B:113:LYS:HD3	2.34	0.48
2:D:485:LEU:HD13	1:B:24:ASP:O	2.14	0.48
1:B:8:LEU:HD13	1:B:101:HIS:HB3	1.96	0.48
2:D:442:LYS:HE2	2:D:445:LYS:HD2	1.96	0.48
2:D:201:ALA:O	2:D:231:MET:HG3	2.14	0.48
2:D:457:GLU:CG	1:B:113:LYS:HZ2	2.25	0.48
2:D:405:ARG:CG	2:D:406:ASN:H	2.25	0.48
1:A:186:THR:OG1	1:A:213:LYS:NZ	2.43	0.48
1:B:282:ILE:O	1:B:285:CYS:HB2	2.13	0.48
2:C:207:ASN:OD1	2:C:208:THR:N	2.46	0.48
2:D:196:THR:O	2:D:200:PHE:HD1	1.97	0.48
2:D:481:SER:C	2:D:483:LYS:H	2.16	0.48
2:D:435:SER:OG	1:B:270:GLU:N	2.45	0.48
2:D:436:GLN:N	2:D:437:PRO:CD	2.77	0.48
1:B:185:LEU:CD2	1:B:260:ALA:HB3	2.43	0.48
1:A:295:ALA:HA	1:A:328:LYS:H	1.78	0.48
2:D:494:LEU:HB3	1:B:56:ASP:CG	2.34	0.47
1:A:282:ILE:O	1:A:285:CYS:HB2	2.14	0.47
2:D:195:GLN:HA	2:D:198:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:O	1:B:342:GLY:HA3	2.13	0.47
2:D:257:MET:CE	2:D:290:LEU:CD1	2.89	0.47
1:A:148:THR:CG2	1:A:167:GLU:OE2	2.62	0.47
2:D:460:SER:HB2	1:B:372:ARG:HD3	1.96	0.47
1:A:137:GLN:HG2	1:A:339:VAL:HG11	1.95	0.47
2:D:280:SER:HA	2:D:283:GLU:HB2	1.96	0.47
2:D:254:LEU:HD22	2:D:285:GLU:HG2	1.97	0.47
2:D:294:THR:CG2	2:D:322:LYS:NZ	2.78	0.47
2:C:264:THR:HA	2:C:295:THR:HG21	1.97	0.47
2:C:231:MET:HE2	2:C:232:LEU:HD23	1.97	0.47
2:D:166:VAL:HG12	2:D:167:ILE:N	2.25	0.47
2:C:166:VAL:HB	2:C:169:ASP:HB3	1.96	0.47
1:B:286:ASP:HB3	1:B:289:ILE:HG12	1.96	0.47
1:B:327:ILE:N	1:B:327:ILE:HD12	2.29	0.47
2:C:230:GLU:HA	2:C:233:LYS:HE2	1.97	0.46
2:C:283:GLU:OE1	2:C:301:TYR:OH	2.32	0.46
1:A:140:LEU:O	1:A:342:GLY:HA3	2.16	0.46
2:C:254:LEU:HB3	2:C:258:ARG:HH21	1.81	0.46
1:B:284:LYS:HB2	1:B:284:LYS:HZ3	1.80	0.46
2:D:329:GLN:HG3	2:D:330:GLU:N	2.30	0.46
2:D:435:SER:CA	2:D:437:PRO:HD3	2.44	0.46
2:D:234:VAL:O	2:D:234:VAL:CG1	2.62	0.46
1:A:50:LYS:HD2	1:A:53:TYR:CE2	2.51	0.46
2:C:187:ASN:HD22	1:B:49:GLN:CB	2.27	0.46
1:A:361:GLU:O	1:A:365:SER:OG	2.33	0.46
2:C:278:MET:HA	2:C:278:MET:HE2	1.98	0.46
2:D:417:ALA:O	2:D:418:GLN:HG2	2.15	0.46
2:C:187:ASN:C	2:C:189:ILE:H	2.18	0.45
1:A:286:ASP:HB3	1:A:289:ILE:HG12	1.96	0.45
1:A:284:LYS:NZ	1:A:284:LYS:CB	2.76	0.45
2:D:178:ASP:C	2:D:180:ASP:H	2.20	0.45
1:A:147:ARG:NH2	1:A:330:ILE:HG12	2.31	0.45
1:B:21:PHE:O	1:B:24:ASP:HB2	2.16	0.45
1:A:185:LEU:CD2	1:A:260:ALA:HB3	2.47	0.45
2:D:208:THR:HA	2:D:237:HIS:CD2	2.51	0.45
2:C:187:ASN:OD1	2:C:187:ASN:O	2.35	0.45
1:B:213:LYS:HA	1:B:217:CYS:SG	2.56	0.45
2:D:172:ASP:O	2:D:176:SER:HB2	2.17	0.45
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.64	0.45
2:D:487:ARG:NH1	1:B:25:ASP:OD2	2.50	0.45
2:C:182:THR:HA	2:C:209:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PRO:HB3	1:B:224:GLU:OE1	2.16	0.45
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.97	0.45
1:B:8:LEU:HD13	1:B:101:HIS:CB	2.47	0.45
1:A:279:TYR:HD1	1:A:294:TYR:HH	1.64	0.45
2:D:396:PRO:HB2	2:D:397:LEU:H	1.63	0.45
1:B:49:GLN:H	1:B:49:GLN:HG2	1.68	0.45
2:C:253:ILE:HG13	2:C:278:MET:SD	2.57	0.45
2:D:232:LEU:CD1	2:D:266:LEU:HD22	2.43	0.45
2:D:224:ALA:O	2:D:227:ALA:HB3	2.17	0.45
1:B:66:THR:HG22	1:B:68:LYS:HE2	1.98	0.45
1:A:34:ILE:HG22	1:A:69:TYR:CE2	2.52	0.45
2:C:189:ILE:O	2:C:190:GLU:C	2.54	0.45
1:B:42:GLY:O	1:B:43:VAL:C	2.54	0.45
1:B:295:ALA:HA	1:B:328:LYS:H	1.82	0.45
2:D:436:GLN:N	2:D:437:PRO:HD3	2.32	0.44
2:D:243:VAL:CG1	2:D:248:ILE:HD12	2.47	0.44
2:D:225:ALA:O	2:D:229:ALA:N	2.45	0.44
1:B:180:LEU:CD1	1:B:267:LEU:CD1	2.94	0.44
2:D:194:THR:HG21	2:D:223:SER:OG	2.17	0.44
2:D:461:ARG:O	2:D:461:ARG:HG3	2.16	0.44
2:D:305:LEU:HA	2:D:306:PRO:HD3	1.86	0.44
1:A:43:VAL:HB	2:D:217:ASN:ND2	2.31	0.44
1:A:64:ILE:HA	1:A:64:ILE:HD13	1.88	0.44
1:A:202:THR:O	1:A:205:GLU:HG2	2.17	0.44
2:D:432:SER:C	2:D:434:GLY:N	2.71	0.44
2:C:281:GLN:O	2:C:285:GLU:HG2	2.16	0.44
2:D:457:GLU:CB	1:B:113:LYS:HD3	2.43	0.44
1:B:190:MET:HG3	1:B:209:VAL:HG21	1.98	0.44
2:D:260:LEU:HA	2:D:263:ASN:HB3	1.97	0.44
1:A:244:ASP:OD1	1:A:244:ASP:N	2.47	0.44
2:C:310:MET:HE2	1:B:115:ASN:OD1	2.17	0.44
2:C:186:LEU:HB3	2:C:191:ASN:HD22	1.83	0.43
2:D:249:THR:CG2	2:D:275:ARG:HH21	2.30	0.43
1:A:47:MET:HE1	1:A:53:TYR:CD1	2.53	0.43
2:D:435:SER:N	1:B:270:GLU:HG2	2.33	0.43
1:A:200:PHE:HA	1:A:205:GLU:CD	2.39	0.43
1:A:47:MET:HE2	1:A:53:TYR:CE1	2.51	0.43
2:C:195:GLN:HA	2:C:198:THR:HB	2.01	0.43
2:D:288:LYS:HG3	2:D:289:LEU:N	2.33	0.43
1:A:219:VAL:HG22	1:A:258:PRO:HB2	2.00	0.43
1:A:242:LEU:HB3	1:A:243:PRO:CD	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:490:VAL:HG21	1:B:30:VAL:HG21	2.00	0.43
2:C:204:LEU:HA	2:C:207:ASN:HB2	2.00	0.43
2:C:213:PHE:CZ	2:C:215:LEU:HD22	2.53	0.43
1:A:221:LEU:CD2	1:A:311:ASP:HB2	2.46	0.43
2:C:271:PHE:CE2	2:C:299:LEU:HD21	2.44	0.43
2:C:254:LEU:HA	2:C:257:MET:HB2	2.00	0.43
2:D:294:THR:HG23	2:D:322:LYS:CD	2.46	0.43
2:C:247:PHE:CD2	2:C:275:ARG:HB3	2.54	0.43
1:B:332:PRO:O	1:B:335:ARG:NH1	2.49	0.43
2:C:175:LYS:H	2:C:175:LYS:HG2	1.60	0.43
1:A:70:PRO:HG3	1:A:81:ASP:HB3	2.00	0.42
2:D:243:VAL:HG13	2:D:248:ILE:CD1	2.49	0.42
2:D:235:ASN:OD1	2:D:236:GLU:N	2.52	0.42
2:D:442:LYS:NZ	1:B:73:HIS:CD2	2.88	0.42
2:D:226:MET:O	2:D:230:GLU:HG2	2.20	0.42
1:B:39:ARG:CB	1:B:64:ILE:O	2.65	0.42
1:A:305:MET:HA	1:A:335:ARG:NH2	2.34	0.42
2:D:221:ASP:C	2:D:221:ASP:OD1	2.56	0.42
2:D:178:ASP:HA	2:D:179:PRO:HD3	1.88	0.42
1:A:31:PHE:CD2	1:A:93:GLU:HG2	2.55	0.42
1:A:210:ARG:NH1	1:A:214:GLU:OE2	2.52	0.42
2:D:192:ILE:HG22	2:D:197:LEU:HG	2.02	0.42
2:D:236:GLU:O	2:D:265:VAL:HG11	2.18	0.42
1:B:291:GLU:HG3	1:B:325:MET:SD	2.60	0.42
1:A:41:GLN:HB3	1:A:42:GLY:H	1.68	0.42
2:D:282:VAL:O	2:D:286:ILE:HG13	2.20	0.42
1:A:351:THR:HG22	2:D:411:ILE:HG22	1.99	0.42
1:B:38:PRO:HD3	1:B:47:MET:CE	2.50	0.42
1:B:218:TYR:CE2	1:B:255:PHE:HB3	2.55	0.42
2:D:432:SER:CB	1:B:178:LEU:HD12	2.49	0.41
2:C:250:GLY:O	2:C:254:LEU:HG	2.19	0.41
2:D:193:THR:HG22	2:D:194:THR:N	2.34	0.41
2:D:254:LEU:HD22	2:D:285:GLU:CG	2.50	0.41
2:C:231:MET:CE	2:C:232:LEU:HD23	2.50	0.41
1:B:286:ASP:OD1	1:B:287:VAL:N	2.53	0.41
1:A:303:THR:O	1:A:303:THR:CG2	2.67	0.41
2:D:199:ARG:HA	2:D:199:ARG:HD3	1.85	0.41
2:C:252:GLY:O	2:C:255:ALA:HB3	2.21	0.41
1:B:134:VAL:HG13	1:B:134:VAL:O	2.20	0.41
2:D:442:LYS:CE	2:D:445:LYS:HB3	2.51	0.41
2:D:322:LYS:O	2:D:326:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:PHE:O	2:D:275:ARG:HD3	2.20	0.41
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.01	0.41
2:D:490:VAL:O	2:D:490:VAL:HG22	2.21	0.41
2:D:482:ILE:O	2:D:482:ILE:HG22	2.21	0.41
2:C:251:LYS:H	2:C:251:LYS:CD	2.34	0.41
1:A:69:TYR:HA	1:A:70:PRO:HD3	1.95	0.41
2:C:287:VAL:HG11	2:C:311:SER:HB3	1.99	0.41
2:D:243:VAL:HG13	2:D:246:ASN:HD22	1.85	0.41
1:A:202:THR:HG23	1:A:205:GLU:OE2	2.21	0.41
1:B:38:PRO:HG3	1:B:47:MET:SD	2.61	0.41
1:A:282:ILE:HG23	1:A:293:LEU:HD23	2.03	0.41
1:A:313:MET:HB3	1:A:329:ILE:CD1	2.51	0.41
1:B:162:THR:HG21	1:B:278:THR:HA	2.03	0.41
2:D:271:PHE:CD2	2:D:271:PHE:N	2.89	0.41
2:C:327:ARG:NH1	1:B:125:GLU:OE2	2.51	0.41
2:D:444:ILE:HG21	1:B:72:GLU:OE1	2.21	0.40
2:C:264:THR:C	2:C:265:VAL:HG22	2.41	0.40
2:D:481:SER:C	2:D:483:LYS:N	2.74	0.40
2:C:217:ASN:HD21	1:B:43:VAL:HA	1.86	0.40
2:C:306:PRO:O	2:C:310:MET:HB2	2.21	0.40
1:A:284:LYS:HB2	1:A:284:LYS:HZ3	1.85	0.40
2:C:324:ARG:HA	2:C:327:ARG:HH12	1.84	0.40
1:B:213:LYS:O	1:B:217:CYS:HB2	2.20	0.40
1:A:47:MET:HE1	1:A:65:LEU:HD21	2.04	0.40
1:B:34:ILE:HD13	1:B:67:LEU:HD13	2.03	0.40

All (2) 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:225:GLN:OE1	2:D:447:SER:O[1_665]	2.15	0.05
1:A:232:SER:O	2:D:432:SER:O[1_665]	2.16	0.04

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	367/384 (96%)	341 (93%)	18 (5%)	8 (2%)	8	36
1	B	367/384 (96%)	346 (94%)	14 (4%)	7 (2%)	10	41
2	C	166/506 (33%)	137 (82%)	23 (14%)	6 (4%)	4	22
2	D	276/506 (54%)	210 (76%)	43 (16%)	23 (8%)	1	4
All	All	1176/1780 (66%)	1034 (88%)	98 (8%)	44 (4%)	4	21

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	45	VAL
2	C	193	THR
2	C	265	VAL
2	D	219	HIS
2	D	390	PRO
2	D	393	PRO
2	D	406	ASN
2	D	436	GLN
2	D	450	SER
1	B	40	HIS
1	B	42	GLY
1	B	43	VAL
1	B	45	VAL
1	A	42	GLY
1	A	44	MET
1	A	182	GLY
2	D	392	PRO
2	D	396	PRO
2	D	401	LYS
2	D	432	SER
2	D	433	VAL
2	D	444	ILE
2	D	446	ASN
1	B	182	GLY
1	A	15	GLY
2	C	191	ASN
2	D	489	GLU
1	A	41	GLN
2	C	275	ARG

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Mol	Chain	Res	Type
2	D	394	PRO
2	D	395	PRO
2	D	421	LEU
2	D	437	PRO
2	D	488	VAL
1	B	15	GLY
1	B	356	TRP
1	A	356	TRP
2	C	188	ASN
2	D	464	THR
2	D	482	ILE
2	D	438	ASN
2	D	462	PRO
2	C	308	PRO

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	311/325 (96%)	282 (91%)	29 (9%)	11	38
1	B	310/325 (95%)	285 (92%)	25 (8%)	15	45
2	C	152/451 (34%)	129 (85%)	23 (15%)	3	15
2	D	241/451 (53%)	213 (88%)	28 (12%)	7	26
All	All	1014/1552 (65%)	909 (90%)	105 (10%)	9	31

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	CYS
1	A	18	LYS
1	A	40	HIS
1	A	44	MET
1	A	49	GLN
1	A	84	LYS
1	A	132	MET

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Mol	Chain	Res	Type
1	A	155	SER
1	A	162	THR
1	A	169	TYR
1	A	175	ILE
1	A	180	LEU
1	A	195	GLU
1	A	196	ARG
1	A	203	THR
1	A	225	GLN
1	A	232	SER
1	A	233	SER
1	A	237	GLU
1	A	281	SER
1	A	288	ASP
1	A	312	ARG
1	A	322	LYS
1	A	334	GLU
1	A	350	SER
1	A	351	THR
1	A	354	GLN
1	A	365	SER
1	A	368	SER
2	C	181	THR
2	C	190	GLU
2	C	196	THR
2	C	198	THR
2	C	215	LEU
2	C	222	ASP
2	C	257	MET
2	C	262	HIS
2	C	265	VAL
2	C	267	THR
2	C	270	ARG
2	C	275	ARG
2	C	281	GLN
2	C	288	LYS
2	C	289	LEU
2	C	292	GLU
2	C	295	THR
2	C	299	LEU
2	C	305	LEU
2	C	310	MET

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Mol	Chain	Res	Type
2	C	313	THR
2	C	318	ARG
2	C	324	ARG
2	D	177	ASN
2	D	206	ASP
2	D	215	LEU
2	D	231	MET
2	D	232	LEU
2	D	243	VAL
2	D	262	HIS
2	D	277	ILE
2	D	280	SER
2	D	282	VAL
2	D	284	MET
2	D	287	VAL
2	D	288	LYS
2	D	289	LEU
2	D	292	GLU
2	D	295	THR
2	D	311	SER
2	D	313	THR
2	D	318	ARG
2	D	404	THR
2	D	407	ILE
2	D	410	VAL
2	D	438	ASN
2	D	445	LYS
2	D	450	SER
2	D	453	GLU
2	D	454	LYS
2	D	456	MET
1	B	17	CYS
1	B	18	LYS
1	B	34	ILE
1	B	40	HIS
1	B	49	GLN
1	B	62	ARG
1	B	84	LYS
1	B	139	VAL
1	B	141	SER
1	B	148	THR
1	B	198	TYR

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Mol	Chain	Res	Type
1	B	201	THR
1	B	227	MET
1	B	232	SER
1	B	236	LEU
1	B	237	GLU
1	B	248	ILE
1	B	287	VAL
1	B	288	ASP
1	B	292	ASP
1	B	303	THR
1	B	336	LYS
1	B	351	THR
1	B	368	SER
1	B	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	78	ASN
2	C	187	ASN
2	C	191	ASN
2	C	261	GLN
2	C	302	HIS
2	D	185	ASN
2	D	207	ASN
2	D	217	ASN
2	D	237	HIS
2	D	246	ASN
2	D	261	GLN
2	D	406	ASN
1	B	73	HIS
1	B	161	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	ANP	A	401	4	29,33,33	2.08	6 (20%)	26,52,52	1.84	4 (15%)
3	ANP	B	401	4	29,33,33	2.12	6 (20%)	26,52,52	1.98	4 (15%)

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
3	ANP	A	401	4	-	0/13/38/38	0/3/3/3
3	ANP	B	401	4	-	0/13/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ANP	C5-C4	2.81	1.46	1.40
3	A	401	ANP	PB-O3A	3.05	1.62	1.59
3	A	401	ANP	C5-C4	3.07	1.47	1.40
3	B	401	ANP	PB-O3A	3.40	1.63	1.59
3	A	401	ANP	PG-N3B	4.23	1.74	1.63
3	B	401	ANP	PB-N3B	4.27	1.75	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ANP	PB-N3B	4.27	1.75	1.63
3	B	401	ANP	PG-N3B	4.41	1.75	1.63
3	A	401	ANP	PB-O1B	4.82	1.51	1.46
3	A	401	ANP	PG-O1G	5.05	1.51	1.46
3	B	401	ANP	PG-O1G	5.19	1.51	1.46
3	B	401	ANP	PB-O1B	5.30	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ANP	N3-C2-N1	-7.53	122.95	128.87
3	A	401	ANP	N3-C2-N1	-6.67	123.63	128.87
3	B	401	ANP	C1'-N9-C4	-2.49	124.03	126.81
3	B	401	ANP	C4'-O4'-C1'	-2.41	107.08	109.64
3	A	401	ANP	C4'-O4'-C1'	-2.32	107.19	109.64
3	A	401	ANP	C1'-N9-C4	-2.13	124.43	126.81
3	A	401	ANP	O2B-PB-O1B	3.47	116.86	110.02
3	B	401	ANP	O2B-PB-O1B	3.67	117.25	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ANP	2	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	369/384 (96%)	0.11	13 (3%) 48 27	22, 39, 61, 94	0
1	B	369/384 (96%)	0.05	6 (1%) 74 54	22, 38, 63, 82	0
2	C	168/506 (33%)	0.37	11 (6%) 22 11	34, 54, 83, 150	0
2	D	280/506 (55%)	1.09	67 (23%) 1 1	34, 61, 184, 280	0
All	All	1186/1780 (66%)	0.36	97 (8%) 14 7	22, 46, 82, 280	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	PRO	8.4
2	D	440	ILE	7.9
2	D	494	LEU	7.5
2	D	431	GLY	7.3
2	D	391	PRO	6.3
2	D	338	ASP	6.0
2	C	197	LEU	5.8
2	D	335	GLU	5.6
2	D	420	ALA	5.5
2	D	423	ASN	5.4
2	D	332	LYS	5.2
2	C	170	ALA	5.0
1	A	42	GLY	4.8
2	D	425	GLN	4.7
2	D	433	VAL	4.6
2	D	432	SER	4.6
2	D	390	PRO	4.5
2	D	439	SER	4.5
2	D	464	THR	4.4
2	D	426	GLY	4.4
2	D	468	SER	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	393	PRO	4.3
2	C	191	ASN	4.2
2	D	424	GLY	4.2
2	D	435	SER	4.2
2	D	430	GLY	4.0
2	D	462	PRO	3.9
2	D	421	LEU	3.9
1	A	45	VAL	3.8
2	D	451	VAL	3.8
2	C	188	ASN	3.8
2	D	457	GLU	3.7
2	D	495	ARG	3.7
1	A	47	MET	3.6
2	D	434	GLY	3.6
2	D	429	SER	3.6
2	D	336	GLY	3.6
2	D	328	LEU	3.6
2	D	441	LEU	3.6
2	D	334	GLN	3.6
1	A	41	GLN	3.5
2	D	392	PRO	3.5
2	D	418	GLN	3.3
1	B	41	GLN	3.3
2	D	458	ASP	3.3
2	D	395	PRO	3.2
2	D	493	ALA	3.2
1	B	201	THR	3.1
2	D	428	GLY	3.1
2	D	437	PRO	3.1
2	D	466	GLN	3.1
2	D	337	TYR	3.1
2	D	465	PRO	3.0
2	D	485	LEU	3.0
1	A	201	THR	3.0
1	A	245	GLY	2.9
2	D	448	LEU	2.9
2	D	331	GLN	2.9
2	C	169	ASP	2.9
2	C	333	GLN	2.9
2	C	193	THR	2.8
2	D	469	ALA	2.8
2	D	427	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	484	GLN	2.7
1	A	46	GLY	2.7
1	A	208	ILE	2.7
1	A	44	MET	2.6
2	D	446	ASN	2.6
2	D	333	GLN	2.6
1	A	39	ARG	2.6
2	D	276	HIS	2.6
2	C	187	ASN	2.6
2	D	454	LYS	2.6
2	D	170	ALA	2.5
2	D	169	ASP	2.5
2	D	438	ASN	2.5
1	B	45	VAL	2.5
2	C	183	GLU	2.5
2	D	492	GLU	2.5
2	D	415	GLU	2.4
2	D	452	GLN	2.4
2	D	394	PRO	2.4
1	B	47	MET	2.4
2	C	199	ARG	2.3
1	B	286	ASP	2.3
2	D	194	THR	2.3
1	B	208	ILE	2.2
1	A	62	ARG	2.2
1	A	202	THR	2.2
2	D	443	GLU	2.1
2	D	442	LYS	2.1
2	D	419	ARG	2.1
2	C	181	THR	2.1
2	D	445	LYS	2.1
1	A	349	LEU	2.0
2	D	422	GLN	2.0
2	D	436	GLN	2.0

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

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ANP	A	401	31/31	0.91	0.17	-0.33	34,43,55,59	0
3	ANP	B	401	31/31	0.90	0.18	-0.49	40,50,60,64	0
4	MG	B	402	1/1	0.87	0.24	-	39,39,39,39	0
4	MG	A	402	1/1	0.87	0.24	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.