



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 4CG7
EMDB ID: : EMD-2510
Title : Cryo-EM of the Sec61-complex bound to the idle 80S ribosome
Authors : Gogala, M.; Becker, T.; Beatrix, B.; Barrio-Garcia, C.; Berninghausen, O.; Beckmann, R.
Deposited on : 2013-11-21
Resolution : 6.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

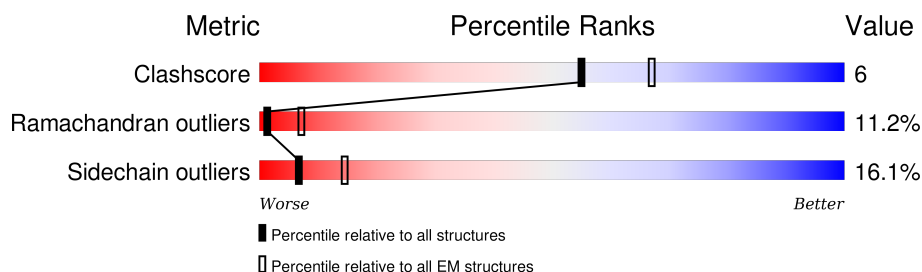
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	476	65% 21% 7% • 5%
2	B	68	76% 13% • 9%
3	C	36	75% 17% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4252 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	452	Total	C	N	O	S	0	0
			3477	2275	560	619	23		

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

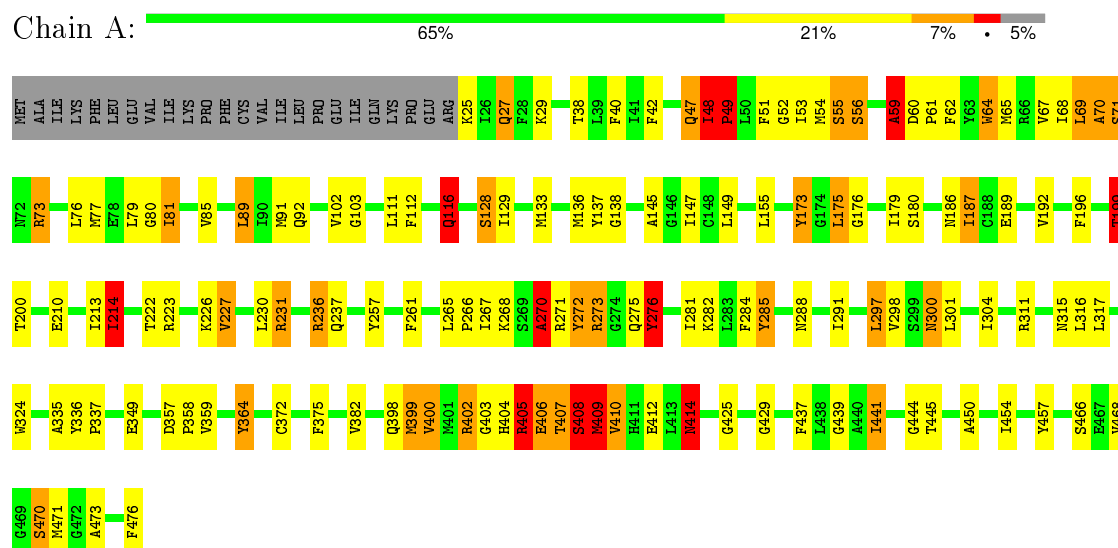
- Molecule 3 is a protein called TRANSPORT PROTEIN SEC61 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	36	Total	C	N	O	S	0	0
			281	188	44	47	2		

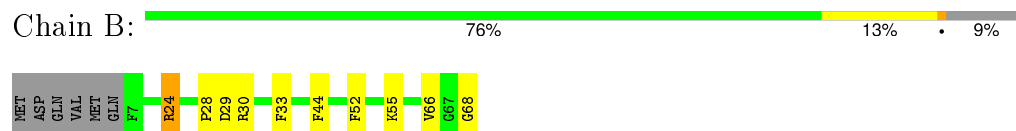
3 Residue-property plots

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. 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. 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.

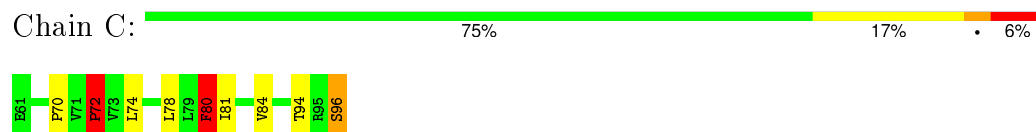
- Molecule 1: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1



- Molecule 2: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA



- Molecule 3: TRANSPORT PROTEIN SEC61 SUBUNIT BETA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided, Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F416 (4K X 4K)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.95	1/3552 (0.0%)	1.30	40/4815 (0.8%)
2	B	1.14	1/504 (0.2%)	1.12	1/673 (0.1%)
3	C	1.33	2/289 (0.7%)	1.36	5/391 (1.3%)
All	All	1.00	4/4345 (0.1%)	1.28	46/5879 (0.8%)

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	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68	GLY	C-O	-14.51	1.00	1.23
1	A	476	PHE	C-O	-12.08	1.00	1.23
3	C	96	SER	C-OXT	-12.07	1.00	1.23
3	C	96	SER	C-O	-12.06	1.00	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	PRO	CA-N-CD	-12.41	94.12	111.50
1	A	276	TYR	CB-CG-CD1	8.76	126.26	121.00
1	A	48	ILE	C-N-CD	-8.75	101.35	120.60
1	A	276	TYR	CB-CG-CD2	-8.69	115.78	121.00
1	A	257	TYR	CB-CG-CD2	-7.56	116.46	121.00
1	A	173	TYR	CB-CG-CD2	-7.09	116.74	121.00
1	A	364	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	71	SER	N-CA-CB	6.69	120.53	110.50
1	A	128	SER	N-CA-CB	6.67	120.50	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	TYR	CB-CG-CD1	6.65	124.99	121.00
1	A	257	TYR	CB-CG-CD1	6.61	124.97	121.00
1	A	364	TYR	CB-CG-CD1	6.61	124.97	121.00
1	A	56	SER	N-CA-CB	6.58	120.37	110.50
2	B	68	GLY	CA-C-O	-6.44	109.02	120.60
3	C	80	PHE	CB-CG-CD1	6.30	125.21	120.80
1	A	336	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	A	55	SER	N-CA-CB	6.24	119.86	110.50
1	A	27	GLN	N-CA-CB	6.14	121.66	110.60
1	A	414	ASN	N-CA-CB	6.01	121.42	110.60
1	A	272	TYR	N-CA-CB	6.00	121.41	110.60
1	A	375	PHE	CB-CG-CD1	6.00	125.00	120.80
1	A	40	PHE	CB-CG-CD1	5.83	124.88	120.80
1	A	336	TYR	CB-CG-CD1	5.75	124.45	121.00
1	A	437	PHE	CB-CG-CD1	5.75	124.82	120.80
1	A	136	MET	N-CA-CB	5.69	120.84	110.60
3	C	80	PHE	CB-CG-CD2	-5.68	116.82	120.80
3	C	80	PHE	CB-CA-C	5.62	121.63	110.40
1	A	272	TYR	N-CA-C	-5.61	95.86	111.00
1	A	61	PRO	C-N-CA	5.52	135.50	121.70
1	A	375	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	A	173	TYR	N-CA-CB	5.50	120.50	110.60
1	A	49	PRO	N-CA-C	5.47	126.32	112.10
1	A	457	TYR	CB-CG-CD1	5.47	124.28	121.00
1	A	116	GLN	N-CA-CB	5.43	120.38	110.60
1	A	270	ALA	N-CA-CB	5.37	117.62	110.10
1	A	40	PHE	CB-CG-CD2	-5.37	117.04	120.80
3	C	72	PRO	N-CA-C	5.35	126.02	112.10
1	A	437	PHE	CB-CG-CD2	-5.33	117.07	120.80
3	C	96	SER	CA-C-O	-5.29	108.99	120.10
1	A	476	PHE	CA-C-O	-5.28	109.02	120.10
1	A	213	ILE	C-N-CA	5.26	134.86	121.70
1	A	59	ALA	N-CA-CB	5.17	117.34	110.10
1	A	67	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	470	SER	N-CA-CB	5.12	118.18	110.50
1	A	49	PRO	N-CA-CB	5.09	109.41	103.30
1	A	137	TYR	C-N-CA	5.04	132.89	122.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	MET	Peptide
1	A	176	GLY	Peptide
1	A	266	PRO	Peptide
1	A	273	ARG	Peptide
1	A	285	TYR	Sidechain
1	A	357	ASP	Peptide
1	A	358	PRO	Peptide
1	A	47	GLN	Peptide
1	A	48	ILE	Peptide
1	A	59	ALA	Peptide
1	A	64	TRP	Peptide
1	A	70	ALA	Peptide
1	A	73	ARG	Sidechain

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	3477	0	3575	56	0
2	B	494	0	527	1	0
3	C	281	0	294	2	0
All	All	4252	0	4396	56	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 6.

All (56) 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:405:ARG:HB3	1:A:408:SER:CB	1.28	1.56
1:A:405:ARG:HB3	1:A:408:SER:OG	1.28	1.32
1:A:405:ARG:CB	1:A:408:SER:CB	2.20	1.19
1:A:405:ARG:HB3	1:A:408:SER:HB2	1.21	1.08
1:A:408:SER:O	1:A:409:MET:HG2	1.53	1.06
1:A:402:ARG:NE	1:A:409:MET:O	1.88	1.06
1:A:402:ARG:CZ	1:A:409:MET:O	2.05	1.05
1:A:405:ARG:CB	1:A:408:SER:OG	2.08	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:CB	1:A:408:SER:HB2	1.87	1.00
1:A:402:ARG:NH2	1:A:409:MET:O	1.93	0.99
1:A:405:ARG:HD3	1:A:408:SER:OG	1.68	0.91
1:A:405:ARG:CA	1:A:408:SER:HB2	2.06	0.85
1:A:408:SER:C	1:A:410:VAL:H	1.80	0.80
1:A:405:ARG:CD	1:A:408:SER:OG	2.30	0.78
1:A:405:ARG:O	1:A:406:GLU:HB2	1.87	0.74
1:A:291:ILE:HD13	1:A:425:GLY:O	1.90	0.71
1:A:405:ARG:C	1:A:408:SER:HB2	2.10	0.71
1:A:408:SER:C	1:A:410:VAL:N	2.46	0.68
1:A:408:SER:O	1:A:409:MET:CG	2.38	0.68
1:A:69:LEU:HD21	1:A:80:GLY:H	1.59	0.67
1:A:408:SER:O	1:A:410:VAL:N	2.30	0.65
1:A:410:VAL:O	1:A:414:ASN:OD1	2.16	0.63
1:A:400:VAL:HG13	1:A:403:GLY:H	1.64	0.62
1:A:406:GLU:O	1:A:409:MET:SD	2.60	0.60
1:A:405:ARG:CG	1:A:408:SER:OG	2.52	0.58
1:A:291:ILE:HD11	1:A:429:GLY:H	1.69	0.57
1:A:405:ARG:HB3	1:A:408:SER:HB3	1.66	0.56
1:A:404:HIS:O	1:A:408:SER:HB3	2.07	0.53
1:A:291:ILE:HD12	1:A:372:CYS:HB3	1.92	0.52
1:A:268:LYS:HB2	1:A:400:VAL:HG11	1.91	0.51
1:A:399:MET:O	1:A:400:VAL:HG12	2.11	0.50
1:A:406:GLU:C	1:A:408:SER:N	2.65	0.50
1:A:441:ILE:HG12	1:A:444:GLY:H	1.75	0.50
1:A:410:VAL:O	1:A:414:ASN:HB3	2.13	0.49
1:A:64:TRP:CZ2	1:A:300:ASN:HB2	2.49	0.48
1:A:291:ILE:HD11	1:A:429:GLY:N	2.29	0.47
1:A:68:ILE:HG23	1:A:85:VAL:CG1	2.44	0.47
1:A:406:GLU:C	1:A:408:SER:H	2.17	0.47
1:A:187:ILE:HB	1:A:450:ALA:HB1	1.98	0.46
1:A:405:ARG:HD3	1:A:408:SER:HG	1.77	0.45
1:A:214:ILE:H	1:A:214:ILE:HD13	1.82	0.45
1:A:64:TRP:CH2	1:A:300:ASN:HB2	2.52	0.45
1:A:408:SER:HB3	1:A:409:MET:H	1.60	0.44
1:A:48:ILE:HG22	3:C:80:PHE:CE1	2.53	0.44
1:A:89:LEU:HD13	1:A:297:LEU:HD23	2.01	0.43
1:A:270:ALA:HB3	1:A:276:TYR:HB3	2.01	0.43
1:A:38:THR:HG22	1:A:42:PHE:CZ	2.54	0.43
1:A:210:GLU:HB2	2:B:52:PHE:CE1	2.55	0.42
1:A:199:THR:HB	1:A:200:THR:H	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG23	1:A:85:VAL:HG13	2.03	0.41
1:A:91:MET:HA	1:A:116:GLN:HE22	1.86	0.41
1:A:53:ILE:HD13	3:C:96:SER:H	1.86	0.41
1:A:407:THR:O	1:A:410:VAL:HG12	2.20	0.40
1:A:410:VAL:O	1:A:414:ASN:CB	2.70	0.40
1:A:410:VAL:O	1:A:414:ASN:CG	2.59	0.40
1:A:405:ARG:CB	1:A:408:SER:HB3	2.38	0.40

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 PDB entries followed by that with respect to all EM entries.

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	450/476 (94%)	356 (79%)	41 (9%)	53 (12%)	0	9
2	B	60/68 (88%)	51 (85%)	4 (7%)	5 (8%)	1	18
3	C	34/36 (94%)	27 (79%)	4 (12%)	3 (9%)	1	17
All	All	544/580 (94%)	434 (80%)	49 (9%)	61 (11%)	1	10

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	49	PRO
1	A	54	MET
1	A	55	SER
1	A	56	SER
1	A	62	PHE
1	A	71	SER
1	A	81	ILE
1	A	102	VAL
1	A	138	GLY

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Mol	Chain	Res	Type
1	A	147	ILE
1	A	149	LEU
1	A	173	TYR
1	A	175	LEU
1	A	199	THR
1	A	214	ILE
1	A	222	THR
1	A	227	VAL
1	A	272	TYR
1	A	316	LEU
1	A	335	ALA
1	A	400	VAL
1	A	412	GLU
1	A	468	VAL
1	A	470	SER
1	A	473	ALA
2	B	24	ARG
2	B	30	ARG
3	C	70	PRO
3	C	72	PRO
1	A	59	ALA
1	A	237	GLN
1	A	273	ARG
1	A	359	VAL
1	A	408	SER
1	A	409	MET
1	A	471	MET
2	B	66	VAL
1	A	70	ALA
1	A	145	ALA
1	A	231	ARG
1	A	270	ALA
1	A	317	LEU
1	A	349	GLU
1	A	398	GLN
1	A	405	ARG
1	A	406	GLU
1	A	466	SER
2	B	29	ASP
3	C	94	THR
1	A	271	ARG
1	A	315	ASN

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Mol	Chain	Res	Type
1	A	226	LYS
1	A	236	ARG
1	A	337	PRO
1	A	382	VAL
1	A	439	GLY
1	A	51	PHE
1	A	103	GLY
1	A	52	GLY
2	B	28	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 PDB entries followed by that with respect to all EM entries.

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	375/398 (94%)	311 (83%)	64 (17%)	2	17
2	B	53/59 (90%)	49 (92%)	4 (8%)	17	53
3	C	32/32 (100%)	26 (81%)	6 (19%)	2	13
All	All	460/489 (94%)	386 (84%)	74 (16%)	7	20

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	29	LYS
1	A	47	GLN
1	A	49	PRO
1	A	60	ASP
1	A	65	MET
1	A	69	LEU
1	A	73	ARG
1	A	76	LEU
1	A	77	MET
1	A	79	LEU
1	A	81	ILE
1	A	89	LEU

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Mol	Chain	Res	Type
1	A	92	GLN
1	A	111	LEU
1	A	112	PHE
1	A	116	GLN
1	A	128	SER
1	A	129	ILE
1	A	155	LEU
1	A	175	LEU
1	A	179	ILE
1	A	180	SER
1	A	186	ASN
1	A	187	ILE
1	A	189	GLU
1	A	192	VAL
1	A	196	PHE
1	A	199	THR
1	A	214	ILE
1	A	223	ARG
1	A	227	VAL
1	A	230	LEU
1	A	231	ARG
1	A	236	ARG
1	A	261	PHE
1	A	265	LEU
1	A	267	ILE
1	A	275	GLN
1	A	276	TYR
1	A	281	ILE
1	A	282	LYS
1	A	284	PHE
1	A	285	TYR
1	A	288	ASN
1	A	297	LEU
1	A	298	VAL
1	A	300	ASN
1	A	301	LEU
1	A	304	ILE
1	A	311	ARG
1	A	324	TRP
1	A	364	TYR
1	A	399	MET
1	A	402	ARG

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Mol	Chain	Res	Type
1	A	405	ARG
1	A	407	THR
1	A	408	SER
1	A	409	MET
1	A	410	VAL
1	A	414	ASN
1	A	441	ILE
1	A	445	THR
1	A	454	ILE
2	B	24	ARG
2	B	33	PHE
2	B	44	PHE
2	B	55	LYS
3	C	72	PRO
3	C	74	LEU
3	C	78	LEU
3	C	80	PHE
3	C	81	ILE
3	C	84	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	244	ASN
2	B	58	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.