



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3J15
EMDB ID: : EMD-2009
Title : Model of ribosome-bound archaeal Pelota and ABCE1
Authors : Becker, T.; Franckenberg, S.; Wickles, S.; Shoemaker, C.J.; Anger, A.M.;
Armache, J.-P.; Sieber, H.; Ungewickell, C.; Berninghausen, O.; Daberkow, I.;
Karcher, A.; Thomm, M.; Hopfner, K.-P.; Green, R.; Beckmann, R.
Deposited on : 2011-12-12
Resolution : 6.60 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 : 1.7.1 (RC1), CSD as537be (2016)
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

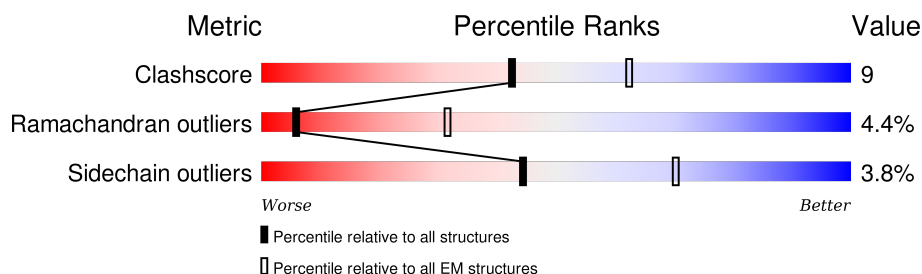
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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)	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	357	
2	B	593	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	B	601	-	-	X	-
3	ADP	B	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7660 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 pelota.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	357	2861	1818	503	533	7	0	0

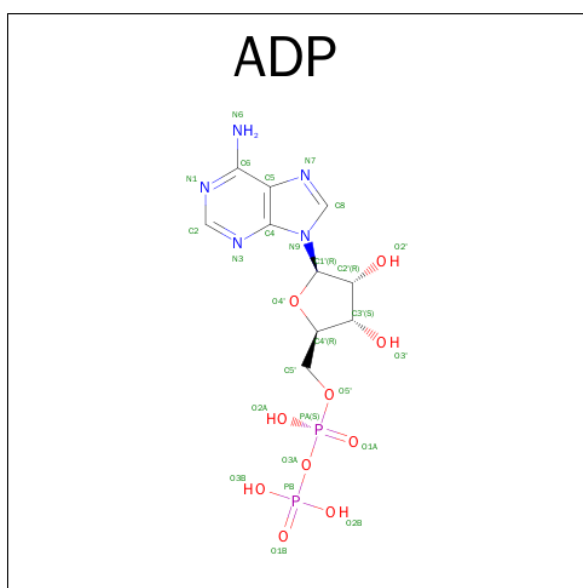
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	GLN	ENGINEERED MUTATION	UNP Q5JIB9

- Molecule 2 is a protein called ABC transporter ATP-binding protein.

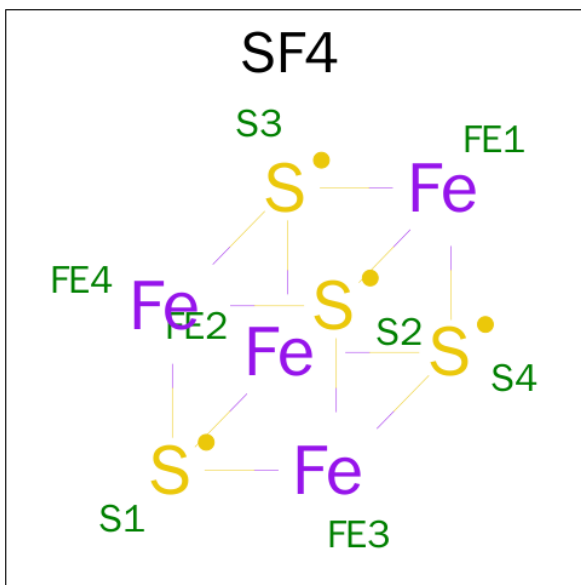
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	593	4729	3003	826	880	20	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
3	B	1	Total	C	N	O	P	0
			54	20	10	20	4	

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

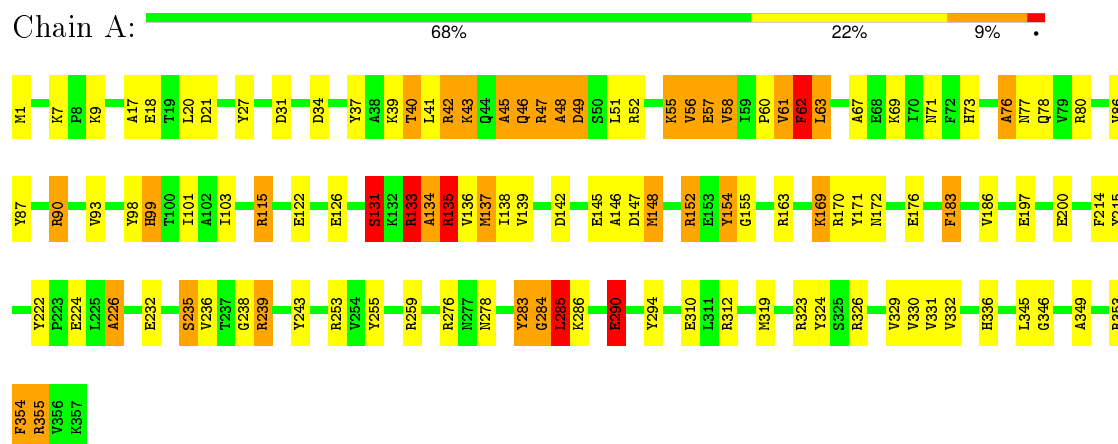


Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	Fe	S	0
			16	8	8	
4	B	1	Total	Fe	S	0
			16	8	8	

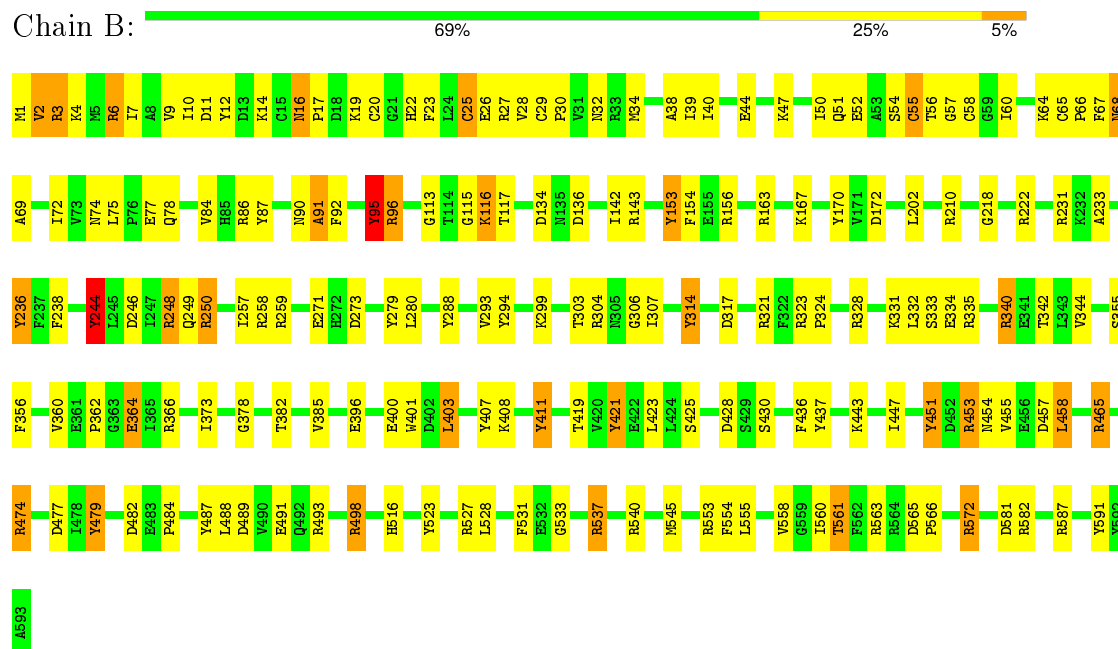
3 Residue-property plots

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 pelota



• Molecule 2: ABC transporter ATP-binding protein



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	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ADP

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	1.72	33/2903 (1.1%)	2.05	83/3904 (2.1%)
2	B	1.66	43/4815 (0.9%)	1.89	106/6499 (1.6%)
All	All	1.68	76/7718 (1.0%)	1.95	189/10403 (1.8%)

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	11
2	B	0	19
All	All	0	30

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	ARG	CD-NE	8.13	1.60	1.46
2	B	453	ARG	NE-CZ	7.92	1.43	1.33
1	A	154	TYR	CG-CD1	7.66	1.49	1.39
1	A	353	ARG	CZ-NH2	7.02	1.42	1.33
1	A	253	ARG	CZ-NH2	6.93	1.42	1.33
2	B	563	ARG	CD-NE	6.93	1.58	1.46
2	B	154	PHE	CE2-CZ	6.93	1.50	1.37
2	B	540	ARG	NE-CZ	6.77	1.41	1.33
2	B	294	TYR	CZ-OH	6.62	1.49	1.37
2	B	453	ARG	CZ-NH1	6.53	1.41	1.33
2	B	294	TYR	CE1-CZ	6.40	1.46	1.38
2	B	430	SER	CA-CB	6.35	1.62	1.52
1	A	312	ARG	CZ-NH1	6.24	1.41	1.33
2	B	484	PRO	CA-C	-6.22	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ASP	N-CA	-6.18	1.33	1.46
2	B	279	TYR	CE2-CZ	6.15	1.46	1.38
1	A	131	SER	CA-CB	6.06	1.62	1.52
2	B	288	TYR	CG-CD2	6.03	1.47	1.39
2	B	537	ARG	NE-CZ	6.00	1.40	1.33
2	B	582	ARG	NE-CZ	5.94	1.40	1.33
2	B	335	ARG	CZ-NH2	5.92	1.40	1.33
1	A	259	ARG	CD-NE	5.91	1.56	1.46
2	B	328	ARG	NE-CZ	5.87	1.40	1.33
1	A	215	TYR	CG-CD1	5.86	1.46	1.39
2	B	360	VAL	CA-CB	-5.86	1.42	1.54
1	A	98	TYR	CD2-CE2	5.86	1.48	1.39
1	A	122	GLU	CB-CG	5.85	1.63	1.52
1	A	253	ARG	CD-NE	5.85	1.56	1.46
2	B	421	TYR	CD1-CE1	5.85	1.48	1.39
2	B	323	ARG	CZ-NH2	5.84	1.40	1.33
2	B	340	ARG	CZ-NH1	5.80	1.40	1.33
2	B	170	TYR	CG-CD1	5.80	1.46	1.39
1	A	126	GLU	CB-CG	5.70	1.62	1.52
1	A	294	TYR	CE2-CZ	5.67	1.46	1.38
1	A	235	SER	CA-CB	5.62	1.61	1.52
2	B	323	ARG	CZ-NH1	5.61	1.40	1.33
1	A	145	GLU	CD-OE2	5.59	1.31	1.25
2	B	222	ARG	CZ-NH1	5.59	1.40	1.33
2	B	364	GLU	CD-OE2	5.59	1.31	1.25
1	A	93	VAL	CB-CG1	5.52	1.64	1.52
2	B	465	ARG	NE-CZ	5.51	1.40	1.33
1	A	80	ARG	CZ-NH2	5.47	1.40	1.33
1	A	37	TYR	N-CA	-5.46	1.35	1.46
1	A	200	GLU	CG-CD	5.43	1.60	1.51
2	B	233	ALA	N-CA	-5.43	1.35	1.46
1	A	330	VAL	CB-CG2	5.42	1.64	1.52
2	B	531	PHE	CB-CG	5.39	1.60	1.51
1	A	312	ARG	CZ-NH2	5.38	1.40	1.33
2	B	334	GLU	CB-CG	5.37	1.62	1.52
2	B	304	ARG	NE-CZ	5.37	1.40	1.33
2	B	96	ARG	CZ-NH1	5.34	1.40	1.33
1	A	215	TYR	CE1-CZ	5.31	1.45	1.38
1	A	87	TYR	CZ-OH	5.31	1.46	1.37
1	A	152	ARG	CZ-NH2	5.27	1.39	1.33
1	A	224	GLU	CG-CD	5.24	1.59	1.51
2	B	591	TYR	CE1-CZ	5.23	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	537	ARG	CD-NE	5.22	1.55	1.46
1	A	238	GLY	CA-C	-5.20	1.43	1.51
2	B	236	TYR	CB-CG	-5.17	1.43	1.51
2	B	92	PHE	CB-CG	-5.17	1.42	1.51
2	B	86	ARG	NE-CZ	5.16	1.39	1.33
1	A	133	ARG	CZ-NH2	5.15	1.39	1.33
1	A	170	ARG	NE-CZ	5.14	1.39	1.33
2	B	498	ARG	CZ-NH2	5.13	1.39	1.33
2	B	411	TYR	CE2-CZ	5.12	1.45	1.38
2	B	306	GLY	N-CA	-5.12	1.38	1.46
2	B	400	GLU	CA-CB	5.12	1.65	1.53
2	B	523	TYR	CE2-CZ	5.11	1.45	1.38
2	B	572	ARG	CZ-NH1	5.11	1.39	1.33
1	A	115	ARG	CZ-NH1	5.08	1.39	1.33
2	B	271	GLU	CB-CG	5.07	1.61	1.52
1	A	278	ASN	CB-CG	5.03	1.62	1.51
2	B	314	TYR	CZ-OH	5.02	1.46	1.37
2	B	582	ARG	CZ-NH1	5.01	1.39	1.33
1	A	27	TYR	CG-CD2	5.00	1.45	1.39
1	A	87	TYR	CE2-CZ	5.00	1.45	1.38

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH1	15.93	128.27	120.30
1	A	98	TYR	CB-CG-CD1	15.88	130.53	121.00
1	A	253	ARG	NE-CZ-NH1	15.54	128.07	120.30
1	A	239	ARG	NE-CZ-NH1	-15.17	112.71	120.30
2	B	453	ARG	NE-CZ-NH1	-14.70	112.95	120.30
2	B	86	ARG	NE-CZ-NH1	-14.67	112.97	120.30
1	A	214	PHE	CB-CG-CD1	14.27	130.79	120.80
2	B	487	TYR	CB-CG-CD2	-14.16	112.50	121.00
2	B	163	ARG	NE-CZ-NH2	-12.44	114.08	120.30
2	B	210	ARG	NE-CZ-NH2	-12.08	114.26	120.30
2	B	248	ARG	NE-CZ-NH1	-11.97	114.31	120.30
1	A	355	ARG	NE-CZ-NH2	-11.31	114.64	120.30
2	B	210	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	A	170	ARG	NE-CZ-NH2	-11.03	114.78	120.30
2	B	493	ARG	NE-CZ-NH1	-10.81	114.90	120.30
2	B	407	TYR	CB-CG-CD2	-10.73	114.56	121.00
1	A	239	ARG	NE-CZ-NH2	10.62	125.61	120.30
1	A	87	TYR	CB-CG-CD1	-10.51	114.69	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	A	90	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	A	214	PHE	CB-CG-CD2	-9.93	113.85	120.80
1	A	98	TYR	CB-CG-CD2	-9.90	115.06	121.00
2	B	244	TYR	CB-CG-CD2	-9.78	115.13	121.00
2	B	335	ARG	NE-CZ-NH2	-9.65	115.47	120.30
2	B	279	TYR	CB-CG-CD1	-9.63	115.22	121.00
1	A	323	ARG	NE-CZ-NH2	-9.53	115.53	120.30
2	B	340	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	A	226	ALA	N-CA-CB	9.49	123.39	110.10
1	A	259	ARG	NE-CZ-NH2	-9.41	115.59	120.30
2	B	366	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	222	TYR	CB-CG-CD2	9.16	126.50	121.00
2	B	366	ARG	NE-CZ-NH2	-8.41	116.10	120.30
2	B	582	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	87	TYR	CB-CG-CD2	8.31	125.99	121.00
2	B	587	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	B	77	GLU	N-CA-CB	8.20	125.35	110.60
2	B	555	LEU	CB-CG-CD2	8.02	124.64	111.00
2	B	451	TYR	CB-CG-CD2	7.98	125.79	121.00
1	A	324	TYR	CG-CD1-CE1	7.98	127.68	121.30
2	B	477	ASP	CB-CG-OD1	-7.95	111.15	118.30
1	A	354	PHE	CB-CG-CD1	7.77	126.24	120.80
1	A	80	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	B	443	LYS	N-CA-CB	7.68	124.42	110.60
1	A	253	ARG	NE-CZ-NH2	-7.65	116.47	120.30
2	B	531	PHE	CB-CG-CD1	7.65	126.16	120.80
2	B	474	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	B	250	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	B	153	TYR	CB-CG-CD2	-7.46	116.52	121.00
1	A	284	GLY	N-CA-C	7.45	131.73	113.10
2	B	163	ARG	NE-CZ-NH1	7.43	124.02	120.30
2	B	143	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	B	95	TYR	CB-CG-CD2	-7.21	116.67	121.00
2	B	321	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	A	163	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	169	LYS	N-CA-CB	7.09	123.37	110.60
2	B	163	ARG	N-CA-CB	7.09	123.36	110.60
2	B	487	TYR	CB-CG-CD1	7.05	125.23	121.00
1	A	349	ALA	N-CA-CB	7.04	119.96	110.10
1	A	34	ASP	CB-CG-OD2	7.02	124.62	118.30
2	B	437	TYR	CZ-CE2-CD2	7.01	126.11	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	NE-CZ-NH1	7.01	123.80	120.30
2	B	91	ALA	N-CA-CB	7.00	119.90	110.10
1	A	27	TYR	CG-CD1-CE1	6.97	126.88	121.30
2	B	250	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	276	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	B	317	ASP	CB-CG-OD1	-6.93	112.06	118.30
2	B	362	PRO	N-CA-CB	6.89	111.57	103.30
1	A	312	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	80	ARG	NE-CZ-NH1	6.87	123.74	120.30
2	B	479	TYR	CB-CG-CD2	-6.82	116.91	121.00
2	B	451	TYR	CB-CG-CD1	-6.82	116.91	121.00
2	B	259	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	B	271	GLU	OE1-CD-OE2	6.77	131.43	123.30
1	A	57	GLU	CB-CA-C	-6.73	96.94	110.40
2	B	335	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	353	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	139	VAL	CA-CB-CG2	6.64	120.86	110.90
2	B	482	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	319	MET	CG-SD-CE	-6.58	89.68	100.20
2	B	451	TYR	CG-CD2-CE2	6.49	126.49	121.30
2	B	328	ARG	NE-CZ-NH2	6.47	123.53	120.30
2	B	458	LEU	CB-CG-CD1	6.44	121.95	111.00
2	B	400	GLU	OE1-CD-OE2	6.42	131.01	123.30
1	A	27	TYR	CB-CG-CD1	6.38	124.83	121.00
2	B	87	TYR	CG-CD2-CE2	-6.35	116.22	121.30
2	B	537	ARG	NE-CZ-NH1	-6.26	117.17	120.30
2	B	531	PHE	CB-CG-CD2	-6.25	116.42	120.80
2	B	356	PHE	CB-CG-CD1	-6.20	116.46	120.80
1	A	163	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	B	231	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	B	523	TYR	CB-CG-CD2	-6.12	117.33	121.00
2	B	244	TYR	CB-CG-CD1	6.10	124.66	121.00
2	B	482	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	46	GLN	CA-CB-CG	6.07	126.76	113.40
2	B	163	ARG	N-CA-C	-6.06	94.63	111.00
1	A	324	TYR	CD1-CE1-CZ	-6.04	114.37	119.80
2	B	553	ARG	NE-CZ-NH1	6.03	123.32	120.30
2	B	488	LEU	CB-CG-CD2	6.02	121.23	111.00
1	A	283	TYR	CA-CB-CG	6.01	124.82	113.40
2	B	527	ARG	N-CA-CB	6.00	121.41	110.60
1	A	148	MET	N-CA-CB	6.00	121.40	110.60
2	B	328	ARG	CG-CD-NE	-6.00	99.21	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	TYR	CB-CG-CD2	5.99	124.60	121.00
1	A	326	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	B	396	GLU	CB-CA-C	-5.98	98.44	110.40
1	A	135	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	48	ALA	N-CA-CB	5.94	118.42	110.10
2	B	561	THR	CA-CB-CG2	-5.94	104.08	112.40
1	A	283	TYR	CB-CG-CD2	5.94	124.56	121.00
1	A	45	ALA	CB-CA-C	-5.91	101.24	110.10
2	B	385	VAL	CG1-CB-CG2	-5.83	101.57	110.90
1	A	62	PHE	CB-CG-CD2	-5.83	116.72	120.80
2	B	533	GLY	N-CA-C	-5.83	98.54	113.10
1	A	93	VAL	CA-CB-CG1	-5.82	102.16	110.90
1	A	67	ALA	N-CA-CB	5.79	118.21	110.10
1	A	284	GLY	C-N-CA	5.77	136.12	121.70
1	A	134	ALA	N-CA-CB	5.76	118.16	110.10
1	A	17	ALA	CB-CA-C	-5.74	101.49	110.10
1	A	18	GLU	OE1-CD-OE2	5.74	130.18	123.30
2	B	477	ASP	CB-CG-OD2	5.72	123.45	118.30
2	B	84	VAL	CG1-CB-CG2	-5.71	101.77	110.90
2	B	436	PHE	CB-CG-CD1	-5.70	116.81	120.80
2	B	489	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	B	288	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	145	GLU	CB-CA-C	-5.68	99.05	110.40
1	A	222	TYR	CB-CG-CD1	-5.66	117.60	121.00
1	A	290	GLU	N-CA-CB	-5.66	100.41	110.60
1	A	283	TYR	CG-CD1-CE1	5.65	125.82	121.30
2	B	288	TYR	CG-CD2-CE2	-5.61	116.81	121.30
1	A	133	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	103	ILE	CB-CA-C	5.59	122.78	111.60
2	B	288	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
2	B	238	PHE	CB-CG-CD2	-5.55	116.92	120.80
2	B	403	LEU	CB-CG-CD2	5.53	120.40	111.00
2	B	86	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	A	90	ARG	N-CA-CB	5.51	120.53	110.60
1	A	319	MET	N-CA-CB	5.51	120.53	110.60
2	B	324	PRO	N-CD-CG	5.50	111.45	103.20
2	B	257	ILE	CB-CA-C	5.47	122.55	111.60
1	A	284	GLY	CA-C-O	-5.47	110.75	120.60
2	B	425	SER	N-CA-CB	5.45	118.67	110.50
1	A	142	ASP	CB-CG-OD1	5.43	123.19	118.30
2	B	248	ARG	NE-CZ-NH2	5.43	123.02	120.30
2	B	479	TYR	CB-CG-CD1	5.39	124.23	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	87	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	B	142	ILE	CA-CB-CG2	5.38	121.65	110.90
2	B	258	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	B	437	TYR	N-CA-CB	5.36	120.25	110.60
2	B	465	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	146	ALA	N-CA-C	-5.34	96.58	111.00
1	A	283	TYR	N-CA-CB	5.34	120.21	110.60
1	A	285	LEU	N-CA-CB	5.34	121.08	110.40
2	B	202	LEU	CB-CA-C	-5.32	100.09	110.20
2	B	493	ARG	NH1-CZ-NH2	5.30	125.23	119.40
2	B	565	ASP	CA-C-O	-5.29	108.98	120.10
2	B	373	ILE	N-CA-CB	5.29	122.98	110.80
2	B	537	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	B	572	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	170	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	37	TYR	N-CA-C	-5.23	96.87	111.00
1	A	133	ARG	N-CA-CB	5.23	120.01	110.60
1	A	329	VAL	CG1-CB-CG2	-5.23	102.53	110.90
1	A	294	TYR	CB-CG-CD1	5.23	124.14	121.00
2	B	554	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	A	90	ARG	N-CA-C	-5.21	96.95	111.00
1	A	332	VAL	CG1-CB-CG2	5.18	119.18	110.90
2	B	491	GLU	OE1-CD-OE2	5.17	129.51	123.30
2	B	465	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	273	ASP	N-CA-C	-5.16	97.07	111.00
2	B	116	LYS	N-CA-CB	5.16	119.88	110.60
2	B	451	TYR	CD1-CE1-CZ	5.15	124.43	119.80
1	A	69	LYS	N-CA-C	-5.14	97.11	111.00
2	B	591	TYR	CB-CG-CD1	5.13	124.08	121.00
1	A	186	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	A	326	ARG	N-CA-CB	5.12	119.81	110.60
2	B	95	TYR	CG-CD2-CE2	-5.11	117.21	121.30
2	B	236	TYR	N-CA-CB	5.11	119.79	110.60
1	A	355	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	58	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	A	171	TYR	CB-CG-CD1	-5.08	117.95	121.00
2	B	333	SER	C-N-CA	5.08	134.40	121.70
2	B	236	TYR	CB-CG-CD2	5.08	124.05	121.00
1	A	71	ASN	CB-CA-C	-5.03	100.33	110.40
2	B	95	TYR	CB-CG-CD1	5.03	124.02	121.00
1	A	183	PHE	N-CA-CB	5.03	119.65	110.60
2	B	299	LYS	CA-CB-CG	5.02	124.45	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	HIS	C-N-CA	5.02	134.25	121.70
2	B	273	ASP	N-CA-CB	5.02	119.64	110.60
2	B	545	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	A	147	ASP	Peptide
1	A	154	TYR	Sidechain
1	A	155	GLY	Peptide
1	A	239	ARG	Sidechain
1	A	284	GLY	Peptide
1	A	31	ASP	Peptide
1	A	310	GLU	Peptide
1	A	354	PHE	Sidechain
1	A	355	ARG	Sidechain
1	A	73	HIS	Sidechain
2	B	153	TYR	Sidechain
2	B	156	ARG	Sidechain
2	B	236	TYR	Sidechain
2	B	244	TYR	Sidechain
2	B	248	ARG	Sidechain
2	B	250	ARG	Sidechain
2	B	280	LEU	Peptide
2	B	314	TYR	Sidechain
2	B	340	ARG	Sidechain
2	B	411	TYR	Sidechain
2	B	421	TYR	Sidechain
2	B	451	TYR	Sidechain
2	B	465	ARG	Sidechain
2	B	474	ARG	Sidechain
2	B	479	TYR	Sidechain
2	B	498	ARG	Sidechain
2	B	537	ARG	Sidechain
2	B	572	ARG	Sidechain
2	B	95	TYR	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	2861	0	2947	46	0
2	B	4729	0	4777	96	0
3	B	54	0	24	27	0
4	B	16	0	0	1	0
All	All	7660	0	7748	134	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.

All (134) 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:42:ARG:HB2	1:A:99:HIS:NE2	1.21	1.46
2:B:355:SER:OG	3:B:601:ADP:N3	1.65	1.26
1:A:40:THR:OG1	1:A:101:ILE:HD11	1.38	1.23
2:B:355:SER:OG	3:B:601:ADP:C2	1.92	1.21
1:A:42:ARG:HB2	1:A:99:HIS:CE1	1.76	1.20
1:A:42:ARG:HD2	1:A:99:HIS:CG	1.79	1.17
1:A:40:THR:OG1	1:A:101:ILE:CD1	1.92	1.16
1:A:42:ARG:HD2	1:A:99:HIS:ND1	1.60	1.15
1:A:42:ARG:CB	1:A:99:HIS:NE2	2.11	1.14
2:B:113:GLY:C	3:B:602:ADP:H5'2	1.72	1.09
2:B:113:GLY:H	3:B:602:ADP:PB	1.76	1.09
1:A:42:ARG:HD2	1:A:99:HIS:CE1	1.88	1.07
1:A:40:THR:HG1	1:A:101:ILE:HD11	0.95	1.02
2:B:113:GLY:N	3:B:602:ADP:O1B	1.95	0.99
1:A:346:GLY:HA3	2:B:34:MET:CE	1.95	0.97
2:B:22:HIS:H	2:B:27:ARG:NH1	1.67	0.92
2:B:6:ARG:NH2	2:B:74:ASN:HD21	1.69	0.90
1:A:42:ARG:CD	1:A:99:HIS:CE1	2.55	0.89
2:B:115:GLY:HA2	3:B:602:ADP:O2A	1.71	0.89
1:A:42:ARG:HD2	1:A:99:HIS:CD2	2.10	0.87
1:A:42:ARG:HB2	1:A:99:HIS:CD2	2.10	0.85
1:A:40:THR:OG1	1:A:101:ILE:HD12	1.76	0.83
2:B:4:LYS:HG3	2:B:75:LEU:O	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:GLY:N	3:B:602:ADP:PB	2.50	0.82
1:A:40:THR:HG21	1:A:101:ILE:HG13	1.66	0.77
2:B:113:GLY:CA	3:B:602:ADP:H5'2	2.15	0.77
1:A:346:GLY:HA3	2:B:34:MET:HE3	1.68	0.75
2:B:2:VAL:O	2:B:3:ARG:HB2	1.84	0.75
1:A:42:ARG:CB	1:A:99:HIS:CD2	2.69	0.74
1:A:42:ARG:CD	1:A:99:HIS:ND1	2.47	0.74
2:B:25:CYS:HB3	2:B:39:ILE:HD13	1.68	0.73
2:B:113:GLY:O	3:B:602:ADP:H5'2	1.88	0.73
2:B:6:ARG:CZ	2:B:74:ASN:HD21	2.01	0.72
1:A:42:ARG:CB	1:A:99:HIS:CE1	2.67	0.72
1:A:43:LYS:HB3	1:A:58:VAL:HA	1.73	0.70
1:A:137:MET:H	1:A:138:ILE:HD12	1.55	0.69
2:B:22:HIS:H	2:B:27:ARG:HH12	1.40	0.69
2:B:7:ILE:HD13	2:B:95:TYR:OH	1.94	0.68
1:A:61:VAL:HG12	1:A:62:PHE:H	1.59	0.66
2:B:30:PRO:HD2	4:B:603:SF4:S2	2.36	0.66
2:B:113:GLY:O	3:B:602:ADP:C5'	2.46	0.63
1:A:345:LEU:O	2:B:30:PRO:HB2	1.99	0.63
2:B:113:GLY:HA2	3:B:602:ADP:H5'2	1.80	0.62
2:B:67:PHE:O	2:B:68:ASN:HB2	1.99	0.62
1:A:39:LYS:HA	1:A:62:PHE:HA	1.80	0.62
2:B:378:GLY:N	3:B:601:ADP:O2B	2.34	0.60
2:B:6:ARG:HD2	2:B:55:CYS:O	2.00	0.60
2:B:378:GLY:H	3:B:601:ADP:PB	2.24	0.59
1:A:42:ARG:NE	1:A:99:HIS:CE1	2.70	0.59
2:B:4:LYS:HE2	2:B:74:ASN:HB3	1.85	0.58
2:B:19:LYS:HD3	2:B:67:PHE:HZ	1.66	0.58
2:B:113:GLY:C	3:B:602:ADP:C5'	2.62	0.58
2:B:9:VAL:HG21	2:B:293:VAL:O	2.03	0.57
2:B:10:ILE:HG23	2:B:69:ALA:O	2.05	0.57
2:B:378:GLY:HA2	3:B:601:ADP:PB	2.45	0.57
2:B:22:HIS:H	2:B:27:ARG:HH11	1.50	0.57
2:B:115:GLY:N	3:B:602:ADP:H5'1	2.18	0.56
2:B:54:SER:O	2:B:55:CYS:C	2.44	0.56
2:B:115:GLY:H	3:B:602:ADP:C5'	2.19	0.56
2:B:355:SER:OG	3:B:601:ADP:H2	1.78	0.55
2:B:40:ILE:HD12	2:B:51:GLN:OE1	2.06	0.55
1:A:43:LYS:HG2	1:A:58:VAL:HG22	1.88	0.54
2:B:6:ARG:NH2	2:B:74:ASN:ND2	2.49	0.54
2:B:6:ARG:CZ	2:B:74:ASN:ND2	2.70	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLY:CA	3:B:602:ADP:O2A	2.52	0.53
2:B:28:VAL:CG1	2:B:60:ILE:HG22	2.40	0.52
2:B:38:ALA:HA	2:B:54:SER:HB2	1.90	0.52
1:A:56:VAL:HG12	1:A:57:GLU:H	1.75	0.52
2:B:16:ASN:C	2:B:16:ASN:HD22	2.13	0.51
2:B:26:GLU:CG	2:B:32:ASN:HD22	2.23	0.51
1:A:346:GLY:HA3	2:B:34:MET:HE1	1.86	0.50
1:A:42:ARG:CD	1:A:99:HIS:CG	2.73	0.50
2:B:4:LYS:HA	2:B:75:LEU:O	2.13	0.48
2:B:4:LYS:CG	2:B:75:LEU:O	2.57	0.48
2:B:453:ARG:HH21	2:B:457:ASP:HB3	1.77	0.48
1:A:346:GLY:HA3	2:B:34:MET:SD	2.53	0.48
2:B:58:CYS:SG	2:B:60:ILE:HG13	2.53	0.48
2:B:382:THR:OG1	3:B:601:ADP:O1B	2.29	0.48
2:B:9:VAL:HG11	2:B:293:VAL:HA	1.95	0.48
1:A:20:LEU:HD13	1:A:77:ASN:HD22	1.78	0.48
1:A:42:ARG:CD	1:A:99:HIS:CD2	2.91	0.48
1:A:285:LEU:HD12	1:A:286:LYS:N	2.29	0.48
2:B:12:TYR:HE1	2:B:90:ASN:O	1.96	0.47
2:B:344:VAL:HG21	2:B:401:TRP:CE3	2.49	0.47
1:A:346:GLY:CA	2:B:34:MET:CE	2.80	0.47
2:B:54:SER:O	2:B:55:CYS:O	2.33	0.47
2:B:423:LEU:HD22	2:B:455:VAL:HG21	1.97	0.47
2:B:39:ILE:HG12	2:B:50:ILE:HG12	1.97	0.47
1:A:43:LYS:HG3	1:A:43:LYS:H	1.41	0.47
2:B:558:VAL:O	2:B:560:ILE:HG12	2.15	0.46
2:B:26:GLU:HG3	2:B:32:ASN:HD22	1.80	0.46
2:B:20:CYS:HB3	2:B:66:PRO:HG3	1.97	0.46
2:B:115:GLY:H	3:B:602:ADP:H5'1	1.79	0.46
2:B:113:GLY:O	3:B:602:ADP:C4'	2.63	0.46
2:B:378:GLY:HA2	3:B:601:ADP:O3A	2.16	0.46
1:A:76:ALA:HB1	1:A:78:GLN:HE21	1.80	0.46
2:B:7:ILE:CD1	2:B:95:TYR:OH	2.64	0.45
2:B:116:LYS:HB2	3:B:602:ADP:O3B	2.16	0.45
1:A:41:LEU:HD21	1:A:58:VAL:HG13	1.99	0.45
2:B:9:VAL:HG22	2:B:91:ALA:O	2.16	0.45
2:B:419:THR:HA	2:B:454:ASN:HA	1.98	0.45
1:A:346:GLY:CA	2:B:34:MET:HE1	2.46	0.44
1:A:135:ARG:HH21	1:A:255:TYR:HB3	1.82	0.44
1:A:133:ARG:HE	1:A:197:GLU:HG3	1.81	0.44
2:B:12:TYR:CE1	2:B:90:ASN:O	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:THR:HG23	2:B:364:GLU:HG3	2.01	0.43
2:B:378:GLY:CA	3:B:601:ADP:O2B	2.67	0.43
1:A:7:LYS:HG3	1:A:9:LYS:H	1.85	0.42
2:B:561:THR:OG1	2:B:581:ASP:HA	2.20	0.42
2:B:28:VAL:HG12	2:B:60:ILE:HG22	2.01	0.42
2:B:65:CYS:HA	2:B:66:PRO:HD2	1.83	0.42
2:B:64:LYS:O	2:B:65:CYS:C	2.57	0.42
2:B:218:GLY:CA	2:B:249:GLN:HE22	2.32	0.42
2:B:11:ASP:OD1	2:B:14:LYS:HE2	2.19	0.42
2:B:344:VAL:HG21	2:B:401:TRP:CD2	2.55	0.42
2:B:10:ILE:CD1	2:B:90:ASN:OD1	2.68	0.42
2:B:12:TYR:C	2:B:14:LYS:H	2.23	0.41
1:A:131:SER:HA	1:A:152:ARG:HG2	2.02	0.41
2:B:17:PRO:HB3	2:B:23:PHE:CE1	2.54	0.41
1:A:47:ARG:CG	1:A:48:ALA:H	2.33	0.41
2:B:218:GLY:HA3	2:B:249:GLN:HE22	1.86	0.41
2:B:29:CYS:HB2	2:B:39:ILE:HD12	2.02	0.41
2:B:378:GLY:CA	3:B:601:ADP:PB	3.08	0.41
2:B:28:VAL:HG11	2:B:64:LYS:HG2	2.01	0.41
2:B:6:ARG:NH2	2:B:56:THR:O	2.54	0.41
2:B:113:GLY:O	3:B:602:ADP:H4'	2.20	0.41
2:B:1:MET:O	2:B:2:VAL:HG13	2.20	0.41
1:A:286:LYS:O	1:A:290:GLU:HB3	2.21	0.41
1:A:346:GLY:C	2:B:34:MET:SD	2.99	0.41
2:B:10:ILE:HA	2:B:69:ALA:O	2.21	0.41
2:B:12:TYR:C	2:B:14:LYS:N	2.74	0.40
2:B:303:THR:O	2:B:307:ILE:HG13	2.21	0.40
2:B:57:GLY:HA2	2:B:72:ILE:HG21	2.03	0.40
1:A:42:ARG:HH11	1:A:42:ARG:HD3	1.74	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	355/357 (99%)	293 (82%)	36 (10%)	26 (7%)	1	21
2	B	591/593 (100%)	524 (89%)	51 (9%)	16 (3%)	6	45
All	All	946/950 (100%)	817 (86%)	87 (9%)	42 (4%)	6	33

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	55	LYS
1	A	60	PRO
1	A	61	VAL
1	A	63	LEU
1	A	131	SER
1	A	137	MET
1	A	148	MET
1	A	176	GLU
1	A	232	GLU
1	A	235	SER
1	A	285	LEU
2	B	3	ARG
2	B	55	CYS
2	B	68	ASN
1	A	45	ALA
1	A	76	ALA
1	A	86	VAL
1	A	99	HIS
1	A	226	ALA
2	B	134	ASP
1	A	49	ASP
1	A	62	PHE
1	A	135	ARG
1	A	169	LYS
1	A	172	ASN
2	B	44	GLU
2	B	428	ASP
1	A	115	ARG
1	A	133	ARG
2	B	25	CYS
2	B	96	ARG
2	B	331	LYS
1	A	134	ALA
2	B	78	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	516	HIS
1	A	136	VAL
2	B	52	GLU
2	B	172	ASP
2	B	244	TYR
2	B	332	LEU
2	B	566	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	305/305 (100%)	287 (94%)	18 (6%)	24	61
2	B	512/512 (100%)	499 (98%)	13 (2%)	55	81
All	All	817/817 (100%)	786 (96%)	31 (4%)	44	73

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	40	THR
1	A	42	ARG
1	A	43	LYS
1	A	47	ARG
1	A	49	ASP
1	A	51	LEU
1	A	52	ARG
1	A	55	LYS
1	A	56	VAL
1	A	62	PHE
1	A	63	LEU
1	A	90	ARG
1	A	183	PHE
1	A	236	VAL
1	A	283	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	290	GLU
1	A	331	VAL
2	B	2	VAL
2	B	6	ARG
2	B	16	ASN
2	B	47	LYS
2	B	117	THR
2	B	136	ASP
2	B	167	LYS
2	B	246	ASP
2	B	403	LEU
2	B	408	LYS
2	B	447	ILE
2	B	458	LEU
2	B	528	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	77	ASN
1	A	78	GLN
1	A	164	HIS
1	A	165	ASN
2	B	16	ASN
2	B	74	ASN
2	B	85	HIS
2	B	249	GLN

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

4 ligands 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$
3	ADP	B	601	-	24,29,29	1.17	3 (12%)	23,45,45	0.89	1 (4%)
3	ADP	B	602	-	24,29,29	1.49	5 (20%)	23,45,45	1.02	1 (4%)
4	SF4	B	603	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	604	2	0,12,12	0.00	-	0,24,24	0.00	-

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	ADP	B	601	-	-	0/12/32/32	0/3/3/3
3	ADP	B	602	-	-	0/12/32/32	0/3/3/3
4	SF4	B	603	2	-	0/0/48/48	0/6/5/5
4	SF4	B	604	2	-	0/0/48/48	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	C8-N7	-2.59	1.29	1.34
3	B	602	ADP	PB-O2B	-2.22	1.47	1.54
3	B	601	ADP	PB-O2B	-2.16	1.47	1.54
3	B	602	ADP	C2-N3	2.15	1.36	1.32
3	B	601	ADP	C4-N3	2.37	1.39	1.35
3	B	601	ADP	PB-O3B	2.94	1.64	1.54
3	B	602	ADP	C4-N3	2.96	1.39	1.35
3	B	602	ADP	PB-O1B	4.14	1.63	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	601	ADP	O2B-PB-O1B	2.08	117.42	110.63
3	B	602	ADP	O3B-PB-O2B	3.02	118.55	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	10	0
3	B	602	ADP	17	0
4	B	603	SF4	1	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.