



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:57 PM GMT

PDB ID : 1I31
Title : MU2 ADAPTIN SUBUNIT (AP50) OF AP2 CLATHRIN ADAPTOR, COM-
PLEXED WITH EGFR INTERNALIZATION PEPTIDE FYRALM AT 2.5
Å RESOLUTION
Authors : Modis, Y.; Boll, W.; Rapoport, I.; Kirchhausen, T.
Deposited on : 2001-02-12
Resolution : 2.50 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

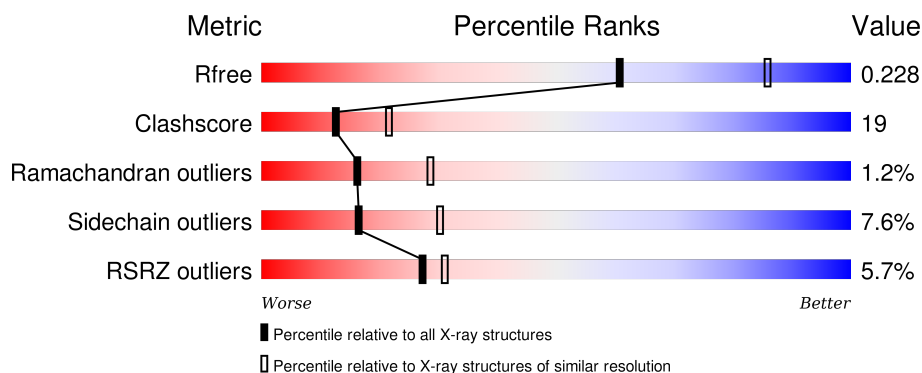
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	314	
2	P	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2169 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 CLATHRIN COAT ASSEMBLY PROTEIN AP50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2066	1327	364	361	14			

- Molecule 2 is a protein called EPIDERMAL GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	S	0	0	0
			56	38	9	8	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	P	3	Total	O	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	125.73 Å 125.73 Å 74.63 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.84 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.50) 96.4 (19.84-2.52)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.53 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.247 , 0.255 0.213 , 0.228	Depositor DCC
R_{free} test set	1123 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.5	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21919 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2169	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

5.1 Standard geometry

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	1.01	2/2107 (0.1%)	2.41	112/2831 (4.0%)
2	P	1.24	0/57	2.66	4/73 (5.5%)
All	All	1.02	2/2164 (0.1%)	2.42	116/2904 (4.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	ARG	CZ-NH2	5.14	1.39	1.33
1	A	323	ARG	NE-CZ	5.08	1.39	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	ARG	NE-CZ-NH2	-20.89	109.86	120.30
1	A	253	ARG	NE-CZ-NH1	20.33	130.47	120.30
1	A	423	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	A	199	ARG	NE-CZ-NH1	15.34	127.97	120.30
1	A	402	ARG	NE-CZ-NH2	-14.87	112.86	120.30
1	A	199	ARG	CD-NE-CZ	14.41	143.78	123.60
1	A	383	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	A	427	ARG	CD-NE-CZ	13.40	142.36	123.60
1	A	423	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	A	219	LYS	C-N-CA	11.80	151.21	121.70
1	A	434	ARG	NE-CZ-NH1	-11.68	114.46	120.30
1	A	288	ARG	NE-CZ-NH1	-11.65	114.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	A	219	LYS	CA-C-O	11.55	144.35	120.10
1	A	427	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	A	218	ASP	CB-CG-OD2	11.23	128.41	118.30
1	A	211	GLU	OE1-CD-OE2	10.57	135.99	123.30
1	A	323	ARG	CD-NE-CZ	-10.36	109.10	123.60
1	A	408	GLU	OE1-CD-OE2	9.78	135.04	123.30
1	A	413	TYR	CB-CG-CD2	9.74	126.85	121.00
1	A	162	ARG	CD-NE-CZ	9.47	136.87	123.60
2	P	1	PHE	CB-CG-CD2	-9.47	114.17	120.80
1	A	162	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	279	THR	CA-CB-CG2	9.30	125.42	112.40
1	A	288	ARG	NE-CZ-NH2	9.29	124.95	120.30
1	A	321	GLU	OE1-CD-OE2	9.25	134.40	123.30
1	A	413	TYR	CB-CG-CD1	-9.20	115.48	121.00
1	A	299	THR	CA-CB-CG2	9.15	125.21	112.40
1	A	415	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	176	ASP	CB-CG-OD2	8.75	126.17	118.30
1	A	269	ASP	CB-CG-OD2	-8.58	110.57	118.30
1	A	323	ARG	NH1-CZ-NH2	8.48	128.73	119.40
1	A	299	THR	N-CA-CB	-8.29	94.55	110.30
1	A	219	LYS	CA-C-N	-8.13	99.30	117.20
1	A	269	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	253	ARG	NH1-CZ-NH2	-7.92	110.69	119.40
1	A	163	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	A	427	ARG	NH1-CZ-NH2	-7.76	110.86	119.40
1	A	334	GLN	CA-CB-CG	7.67	130.27	113.40
2	P	3	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	164	GLU	OE1-CD-OE2	-7.02	114.88	123.30
1	A	164	GLU	CG-CD-OE2	7.01	132.32	118.30
1	A	415	ASP	OD1-CG-OD2	6.90	136.41	123.30
1	A	281	LYS	CD-CE-NZ	6.76	127.25	111.70
1	A	358	MET	CG-SD-CE	-6.72	89.44	100.20
1	A	253	ARG	CD-NE-CZ	6.72	133.01	123.60
1	A	298	ARG	O-C-N	6.72	133.45	122.70
1	A	261	ARG	CD-NE-CZ	6.66	132.93	123.60
1	A	180	SER	N-CA-CB	-6.64	100.54	110.50
1	A	219	LYS	N-CA-CB	6.58	122.44	110.60
1	A	317	ALA	CB-CA-C	-6.58	100.23	110.10
1	A	377	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	357	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	403	TYR	CB-CG-CD1	6.51	124.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	LEU	CB-CA-C	-6.30	98.23	110.20
1	A	209	MET	CG-SD-CE	6.29	110.27	100.20
1	A	164	GLU	C-N-CA	-6.29	109.10	122.30
2	P	1	PHE	CB-CG-CD1	6.23	125.16	120.80
1	A	417	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	180	SER	CB-CA-C	6.18	121.85	110.10
1	A	323	ARG	N-CA-CB	-6.15	99.53	110.60
1	A	339	LYS	CA-CB-CG	6.12	126.86	113.40
1	A	255	SER	N-CA-CB	-6.05	101.43	110.50
1	A	244	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	344	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	A	276	ARG	N-CA-CB	-6.00	99.79	110.60
1	A	415	ASP	O-C-N	-5.99	113.12	122.70
1	A	253	ARG	CG-CD-NE	5.95	124.29	111.80
1	A	169	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	403	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	300	LYS	CA-CB-CG	5.92	126.42	113.40
1	A	321	GLU	CG-CD-OE2	-5.89	106.52	118.30
1	A	317	ALA	N-CA-CB	5.87	118.31	110.10
1	A	177	VAL	CG1-CB-CG2	5.81	120.19	110.90
1	A	434	ARG	NH1-CZ-NH2	5.78	125.75	119.40
1	A	431	TYR	CG-CD2-CE2	-5.71	116.73	121.30
1	A	415	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	278	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	A	339	LYS	CB-CA-C	-5.66	99.08	110.40
1	A	431	TYR	CD1-CE1-CZ	-5.66	114.71	119.80
1	A	301	LEU	N-CA-CB	5.62	121.63	110.40
1	A	211	GLU	CG-CD-OE2	-5.56	107.17	118.30
1	A	191	VAL	CA-CB-CG2	5.52	119.19	110.90
1	A	212	CYS	O-C-N	5.51	131.51	122.70
1	A	336	ILE	CG1-CB-CG2	-5.44	99.43	111.40
1	A	383	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	A	416	HIS	CA-CB-CG	5.41	122.81	113.60
1	A	302	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	206	LEU	O-C-N	5.39	131.32	122.70
1	A	253	ARG	O-C-N	5.37	131.29	122.70
1	A	311	PHE	O-C-N	-5.37	114.11	122.70
1	A	432	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	382	ALA	CB-CA-C	5.30	118.05	110.10
1	A	422	VAL	CB-CA-C	-5.30	101.33	111.40
1	A	197	SER	CB-CA-C	-5.26	100.10	110.10
1	A	188	GLN	CA-CB-CG	5.26	124.96	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	5	LEU	N-CA-C	-5.23	96.89	111.00
1	A	275	MET	CA-C-O	5.22	131.07	120.10
1	A	186	SER	CA-CB-OG	-5.21	97.13	111.20
1	A	371	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	A	266	ILE	N-CA-C	-5.19	97.00	111.00
1	A	402	ARG	C-N-CA	-5.18	108.75	121.70
1	A	432	GLU	CG-CD-OE2	5.16	128.63	118.30
1	A	172	GLU	N-CA-CB	-5.16	101.31	110.60
1	A	316	LEU	CB-CA-C	-5.13	100.45	110.20
1	A	168	TYR	CG-CD1-CE1	5.12	125.40	121.30
1	A	311	PHE	CB-CG-CD1	5.12	124.39	120.80
1	A	295	GLU	OE1-CD-OE2	5.11	129.44	123.30
1	A	183	LEU	CB-CA-C	-5.10	100.51	110.20
1	A	388	MET	CB-CA-C	-5.09	100.22	110.40
1	A	430	ILE	CA-CB-CG1	-5.04	101.42	111.00
1	A	278	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	402	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	A	424	TYR	CD1-CE1-CZ	-5.03	115.28	119.80
1	A	279	THR	CA-CB-OG1	-5.02	98.46	109.00
1	A	431	TYR	CG-CD1-CE1	5.01	125.31	121.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	VAL	Mainchain
1	A	207	SER	Mainchain
1	A	285	LEU	Mainchain
1	A	295	GLU	Mainchain
1	A	312	LYS	Mainchain
1	A	356	LYS	Mainchain

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	2066	0	2158	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	56	0	58	6	0
3	A	44	0	0	5	1
3	P	3	0	0	1	0
All	All	2169	0	2216	84	1

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 19.

All (84) 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:328:LEU:HD12	1:A:328:LEU:H	1.26	1.01
1:A:281:LYS:HZ3	1:A:281:LYS:H	1.04	0.93
1:A:220:ILE:HG12	1:A:242:ALA:HA	1.52	0.90
1:A:281:LYS:NZ	1:A:281:LYS:H	1.81	0.77
1:A:280:THR:H	1:A:281:LYS:HZ2	1.32	0.75
1:A:293:VAL:HG21	1:A:383:ARG:CZ	2.17	0.75
1:A:239:GLN:HB2	1:A:402:ARG:HH22	1.51	0.74
1:A:185:MET:HG3	1:A:190:GLN:O	1.88	0.73
1:A:254:LEU:H	1:A:254:LEU:HD22	1.53	0.72
1:A:328:LEU:N	1:A:328:LEU:HD12	2.02	0.71
1:A:252:VAL:HG13	1:A:263:ILE:HG23	1.72	0.70
1:A:175:LEU:HD11	1:A:404:LEU:HD12	1.73	0.69
1:A:280:THR:OG1	1:A:281:LYS:HD3	1.92	0.69
1:A:422:VAL:HG23	2:P:5:LEU:HB2	1.75	0.68
1:A:244:ASP:OD1	1:A:281:LYS:HE3	1.93	0.67
1:A:328:LEU:CD1	1:A:328:LEU:H	2.05	0.66
1:A:280:THR:H	1:A:281:LYS:NZ	1.95	0.65
1:A:376:ASN:C	1:A:376:ASN:HD22	2.01	0.64
1:A:238:LYS:HE2	1:A:239:GLN:HE21	1.62	0.64
1:A:199:ARG:HD3	3:A:35:HOH:O	1.97	0.64
1:A:219:LYS:HE3	1:A:220:ILE:HB	1.80	0.63
1:A:219:LYS:CE	1:A:219:LYS:HA	2.29	0.62
1:A:239:GLN:OE1	1:A:400:LYS:HE3	2.00	0.61
1:A:248:PHE:HB3	1:A:252:VAL:HG21	1.82	0.61
1:A:207:SER:HB2	1:A:413:TYR:CE2	2.37	0.60
1:A:185:MET:HE1	1:A:288:ARG:HD2	1.83	0.59
1:A:218:ASP:OD1	1:A:220:ILE:HG13	2.03	0.59
1:A:238:LYS:HE2	1:A:239:GLN:NE2	2.17	0.59
1:A:220:ILE:CG1	1:A:242:ALA:HA	2.31	0.59
1:A:185:MET:CE	1:A:288:ARG:HD2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ILE:HD11	1:A:243:ILE:H	1.67	0.57
1:A:337:CYS:HB3	1:A:366:ILE:HG13	1.86	0.57
1:A:311:PHE:O	1:A:312:LYS:C	2.41	0.56
1:A:293:VAL:HG21	1:A:383:ARG:NH1	2.20	0.56
1:A:186:SER:HB2	1:A:187:PRO:HD2	1.88	0.55
1:A:169:ARG:H	1:A:169:ARG:CD	2.19	0.54
1:A:341:LYS:HE2	3:A:26:HOH:O	2.06	0.54
1:A:263:ILE:H	1:A:263:ILE:HD12	1.73	0.54
1:A:268:PRO:HD2	1:A:272:PHE:CE1	2.43	0.54
1:A:422:VAL:CG2	2:P:5:LEU:HB2	2.38	0.54
1:A:376:ASN:HD22	1:A:377:ASP:N	2.06	0.53
1:A:219:LYS:HA	1:A:219:LYS:HE3	1.90	0.53
1:A:331:SER:HB3	1:A:373:LEU:HG	1.92	0.52
1:A:399:LEU:HD23	1:A:400:LYS:N	2.24	0.52
1:A:252:VAL:CG1	1:A:263:ILE:HG23	2.37	0.52
1:A:186:SER:HB2	1:A:187:PRO:CD	2.41	0.51
1:A:220:ILE:CD1	1:A:243:ILE:H	2.25	0.49
1:A:310:ASN:O	1:A:311:PHE:HB3	2.13	0.48
1:A:345:LYS:HD3	1:A:348:GLU:OE2	2.12	0.48
1:A:414:SER:O	1:A:415:ASP:C	2.52	0.48
1:A:403:TYR:CD1	1:A:405:LYS:HG3	2.48	0.48
1:A:263:ILE:N	1:A:263:ILE:HD12	2.29	0.47
1:A:329:ASN:OD1	1:A:329:ASN:N	2.36	0.47
2:P:6:MET:HG2	3:P:15:HOH:O	2.13	0.47
1:A:242:ALA:HB3	1:A:281:LYS:HE2	1.97	0.47
1:A:180:SER:HA	1:A:427:ARG:O	2.14	0.47
1:A:248:PHE:CE2	1:A:263:ILE:HG12	2.49	0.46
1:A:169:ARG:HD2	1:A:169:ARG:H	1.79	0.46
1:A:404:LEU:HD23	1:A:404:LEU:C	2.35	0.46
1:A:323:ARG:HH11	1:A:323:ARG:HD2	1.45	0.46
1:A:185:MET:HE2	3:A:5:HOH:O	2.15	0.46
1:A:323:ARG:HH22	1:A:348:GLU:HB3	1.79	0.46
1:A:279:THR:HG21	1:A:397:SER:HB2	1.97	0.46
1:A:376:ASN:C	1:A:376:ASN:ND2	2.68	0.46
1:A:311:PHE:O	1:A:360:GLY:HA3	2.17	0.45
1:A:253:ARG:HD3	1:A:253:ARG:HA	1.44	0.45
1:A:308:LYS:NZ	1:A:363:GLU:OE2	2.43	0.44
1:A:220:ILE:HG12	1:A:241:ILE:O	2.18	0.44
1:A:304:LYS:NZ	3:A:25:HOH:O	2.50	0.43
1:A:248:PHE:HE2	1:A:263:ILE:HG12	1.83	0.43
1:A:264:SER:O	1:A:265:PHE:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:MET:CE	3:A:5:HOH:O	2.68	0.42
1:A:423:ARG:HB3	2:P:2:TYR:HA	2.01	0.42
1:A:163:ARG:HG2	1:A:166:ILE:HD11	2.01	0.42
1:A:320:ILE:HA	1:A:389:ASN:O	2.20	0.41
1:A:312:LYS:HA	1:A:313:PRO:HD3	1.93	0.41
1:A:239:GLN:HB2	1:A:402:ARG:NH2	2.28	0.41
1:A:238:LYS:CE	1:A:239:GLN:HE21	2.32	0.41
1:A:210:PRO:O	1:A:266:ILE:HA	2.20	0.41
1:A:342:ALA:HA	1:A:352:VAL:O	2.20	0.40
1:A:161:TRP:HH2	1:A:253:ARG:NH2	2.20	0.40
1:A:340:GLY:HA2	1:A:341:LYS:HE3	2.04	0.40
2:P:3:ARG:HA	2:P:3:ARG:HD3	1.84	0.40
1:A:422:VAL:HG21	2:P:5:LEU:HD13	2.03	0.40

All (1) 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)
3:A:1:HOH:O	3:A:1:HOH:O[4_665]	2.05	0.15

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	250/314 (80%)	233 (93%)	14 (6%)	3 (1%)	16	29
2	P	4/6 (67%)	4 (100%)	0	0	100	100
All	All	254/320 (79%)	237 (93%)	14 (6%)	3 (1%)	16	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	LEU
1	A	218	ASP
1	A	219	LYS

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	232/282 (82%)	214 (92%)	18 (8%)	16	29
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	237/287 (83%)	219 (92%)	18 (8%)	16	30

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	180	SER
1	A	184	LEU
1	A	188	GLN
1	A	190	GLN
1	A	219	LYS
1	A	255	SER
1	A	279	THR
1	A	281	LYS
1	A	299	THR
1	A	323	ARG
1	A	328	LEU
1	A	339	LYS
1	A	341	LYS
1	A	376	ASN
1	A	377	ASP
1	A	396	PRO
1	A	408	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/314 (81%)	0.03	13 (5%) 32 36	46, 67, 105, 125	0
2	P	6/6 (100%)	1.01	2 (33%) 0 0	52, 70, 76, 87	0
All	All	262/320 (81%)	0.05	15 (5%) 27 31	46, 67, 103, 125	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	7.6
1	A	239	GLN	6.6
1	A	238	LYS	4.4
2	P	6	MET	3.9
1	A	407	PHE	3.7
1	A	261	ARG	3.6
1	A	260	GLU	3.4
1	A	255	SER	3.0
1	A	382	ALA	2.6
1	A	378	LYS	2.4
1	A	161	TRP	2.3
2	P	1	PHE	2.3
1	A	206	LEU	2.2
1	A	262	SER	2.1
1	A	169	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.