



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 1I31 / pdb_00001i31
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

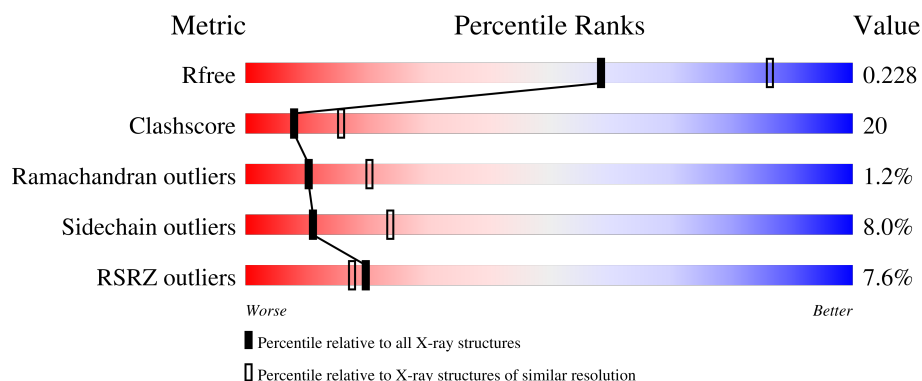
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	6% 31% 35% 13% • 18%
2	P	6	33% 67% 33%

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			

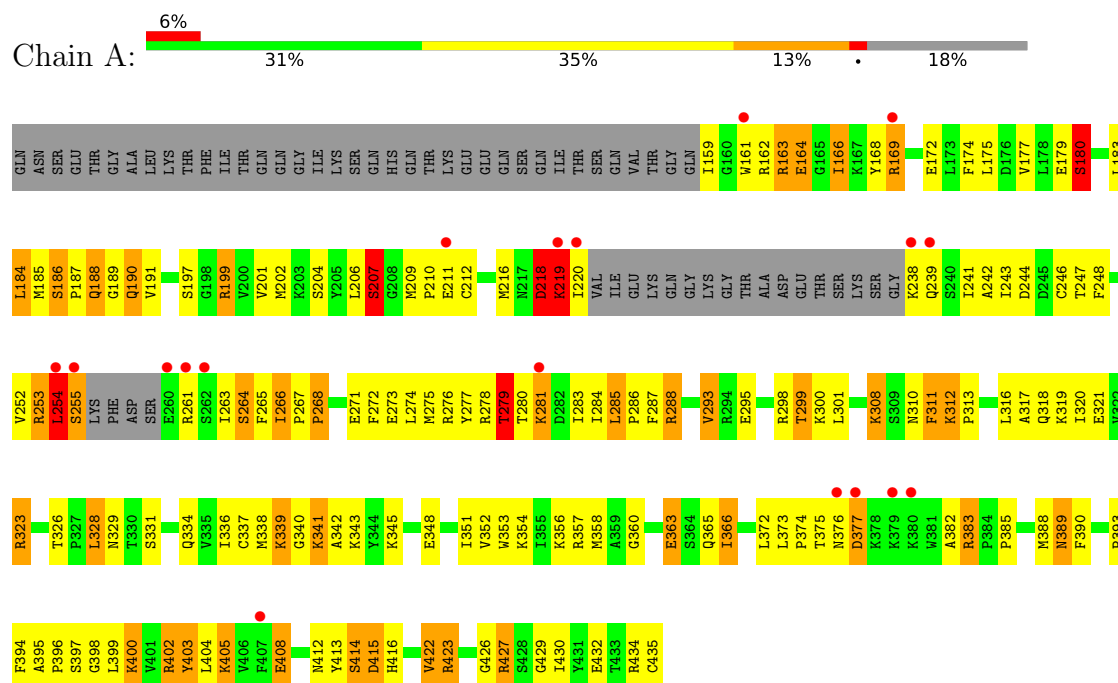
- Molecule 3 is water.

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

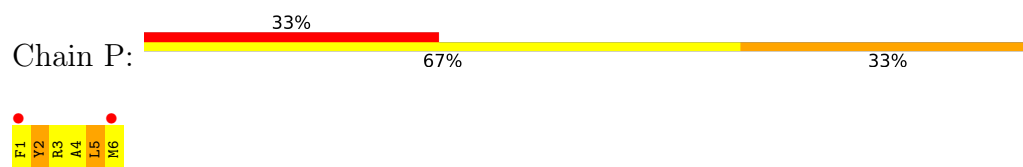
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CLATHRIN COAT ASSEMBLY PROTEIN AP50



• Molecule 2: EPIDERMAL GROWTH FACTOR RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	125.73Å 125.73Å 74.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.50) 96.2 (20.00-2.52)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.53Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.247 , 0.255 0.213 , 0.228	Depositor DCC
R_{free} test set	1123 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 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	1.25	1/2107 (0.0%)	2.74	190/2831 (6.7%)
2	P	1.38	0/57	2.70	6/73 (8.2%)
All	All	1.25	1/2164 (0.0%)	2.74	196/2904 (6.7%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	ARG	NE-CZ	6.00	1.39	1.33

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	CA-C-O	16.67	144.35	120.51
1	A	219	LYS	CA-C-N	16.39	151.21	121.70
1	A	219	LYS	C-N-CA	16.39	151.21	121.70
1	A	199	ARG	CD-NE-CZ	13.84	143.78	124.40
1	A	427	ARG	CD-NE-CZ	12.83	142.36	124.40
1	A	266	ILE	N-CA-C	-11.27	97.00	108.15
1	A	323	ARG	CD-NE-CZ	-10.93	109.10	124.40
1	A	299	THR	N-CA-CB	-10.93	94.55	110.40
1	A	323	ARG	NE-CZ-NH2	-10.38	109.86	119.20
1	A	311	PHE	O-C-N	-9.18	114.11	123.29
1	A	275	MET	CA-C-O	9.14	131.07	121.38
1	A	197	SER	CA-C-N	-9.09	111.85	121.48
1	A	197	SER	C-N-CA	-9.09	111.85	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	HIS	CA-CB-CG	9.01	122.81	113.80
1	A	318	GLN	OE1-CD-NE2	8.99	131.59	122.60
1	A	253	ARG	NE-CZ-NH1	8.97	130.47	121.50
1	A	298	ARG	O-C-N	8.93	133.45	122.20
1	A	162	ARG	CD-NE-CZ	8.90	136.87	124.40
1	A	201	VAL	CA-C-O	-8.79	111.17	120.57
1	A	279	THR	CA-CB-CG2	8.78	125.42	110.50
1	A	299	THR	CA-CB-CG2	8.65	125.21	110.50
1	A	338	MET	CA-C-O	-8.56	111.34	120.42
1	A	267	PRO	CB-CA-C	-8.29	103.38	111.17
1	A	334	GLN	CA-CB-CG	8.08	130.27	114.10
1	A	365	GLN	OE1-CD-NE2	8.07	130.68	122.60
1	A	372	LEU	N-CA-C	7.97	122.23	109.24
1	A	395	ALA	CA-C-O	7.96	125.21	119.32
2	P	4	ALA	CA-C-O	-7.79	112.62	121.19
1	A	184	LEU	CB-CA-C	-7.77	98.23	110.74
1	A	423	ARG	NE-CZ-NH1	7.73	129.23	121.50
1	A	427	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	A	317	ALA	N-CA-C	-7.50	99.72	110.59
1	A	279	THR	CA-CB-OG1	-7.42	98.46	109.60
1	A	253	ARG	CA-C-O	-7.42	112.83	120.84
1	A	390	PHE	CA-C-O	-7.33	113.44	121.28
1	A	317	ALA	CA-C-O	-7.31	113.34	121.89
1	A	323	ARG	NH1-CZ-NH2	7.25	128.73	119.30
1	A	339	LYS	CA-C-O	-7.25	113.03	120.71
1	A	366	ILE	CA-C-O	-7.23	112.57	120.67
1	A	299	THR	CA-CB-OG1	-7.21	98.78	109.60
1	A	415	ASP	O-C-N	-7.12	113.12	122.59
1	A	180	SER	CB-CA-C	7.11	121.85	110.19
1	A	219	LYS	N-CA-CB	7.07	122.44	110.49
2	P	5	LEU	N-CA-C	-7.07	96.89	108.41
1	A	402	ARG	NE-CZ-NH2	-7.04	112.86	119.20
1	A	434	ARG	NE-CZ-NH1	-7.04	114.46	121.50
1	A	288	ARG	NE-CZ-NH1	-7.03	114.47	121.50
1	A	186	SER	CA-CB-OG	-6.99	97.13	111.10
1	A	286	PRO	CA-C-N	-6.95	110.83	122.29
1	A	286	PRO	C-N-CA	-6.95	110.83	122.29
1	A	277	TYR	CA-C-O	6.94	128.83	121.33
1	A	179	GLU	CA-C-O	6.94	129.11	121.06
1	A	284	ILE	CA-C-N	6.89	132.33	121.17
1	A	284	ILE	C-N-CA	6.89	132.33	121.17
1	A	398	GLY	N-CA-C	-6.89	105.00	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ARG	CA-C-O	-6.85	111.87	119.34
1	A	253	ARG	O-C-N	6.85	131.29	122.87
1	A	363	GLU	CA-C-N	-6.82	111.89	122.59
1	A	363	GLU	C-N-CA	-6.82	111.89	122.59
1	A	202	MET	CA-C-O	-6.79	113.03	120.36
1	A	408	GLU	CB-CA-C	6.65	120.19	111.01
2	P	2	TYR	CA-C-O	-6.65	114.31	121.56
1	A	394	PHE	CA-CB-CG	6.63	120.43	113.80
1	A	253	ARG	NH1-CZ-NH2	-6.62	110.69	119.30
1	A	288	ARG	CA-C-O	6.60	127.49	120.36
1	A	323	ARG	N-CA-CB	-6.59	99.53	110.47
1	A	395	ALA	O-C-N	-6.55	115.32	121.35
1	A	212	CYS	O-C-N	6.52	131.51	123.10
1	A	301	LEU	N-CA-CB	6.52	121.63	110.68
1	A	427	ARG	NH1-CZ-NH2	-6.49	110.86	119.30
1	A	402	ARG	CA-C-N	-6.49	108.75	121.91
1	A	402	ARG	C-N-CA	-6.49	108.75	121.91
1	A	199	ARG	NE-CZ-NH1	6.47	127.97	121.50
1	A	385	PRO	CA-C-O	-6.40	113.87	121.67
1	A	288	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	339	LYS	CA-CB-CG	6.38	126.86	114.10
1	A	180	SER	N-CA-CB	-6.38	100.54	110.55
1	A	412	ASN	N-CA-C	6.38	119.73	112.97
1	A	403	TYR	O-C-N	6.30	129.70	123.46
1	A	393	PRO	CA-C-O	-6.30	116.53	121.38
1	A	164	GLU	CA-C-N	-6.28	109.10	121.41
1	A	164	GLU	C-N-CA	-6.28	109.10	121.41
1	A	288	ARG	O-C-N	-6.25	115.86	123.30
1	A	278	ARG	CD-NE-CZ	-6.24	115.66	124.40
1	A	383	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	A	204	SER	CA-C-O	-6.23	113.83	121.11
1	A	206	LEU	O-C-N	6.22	131.32	123.23
1	A	400	LYS	CA-C-N	-6.22	114.34	122.37
1	A	400	LYS	C-N-CA	-6.22	114.34	122.37
1	A	276	ARG	N-CA-CB	-6.19	99.79	111.00
1	A	300	LYS	CA-CB-CG	6.16	126.42	114.10
1	A	253	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	207	SER	CA-C-O	-6.13	114.42	121.47
1	A	246	CYS	N-CA-C	6.09	117.66	108.46
1	A	261	ARG	CD-NE-CZ	6.09	132.93	124.40
1	A	372	LEU	O-C-N	-6.06	116.42	123.27
1	A	164	GLU	CG-CD-OE2	6.05	132.32	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ILE	CA-C-N	-6.03	114.26	122.77
1	A	336	ILE	C-N-CA	-6.03	114.26	122.77
1	A	319	LYS	CA-C-N	-6.01	112.00	121.62
1	A	319	LYS	C-N-CA	-6.01	112.00	121.62
2	P	4	ALA	O-C-N	5.95	130.19	122.87
1	A	278	ARG	O-C-N	-5.90	116.07	123.27
1	A	201	VAL	O-C-N	5.89	129.57	123.03
1	A	183	LEU	N-CA-C	5.88	119.06	109.06
1	A	308	LYS	CA-C-O	-5.87	114.03	120.36
1	A	274	LEU	O-C-N	-5.86	115.76	122.09
1	A	351	ILE	N-CA-C	-5.86	100.14	108.58
1	A	316	LEU	O-C-N	-5.83	115.80	123.21
1	A	317	ALA	O-C-N	5.81	129.48	122.68
1	A	357	ARG	O-C-N	-5.79	115.62	123.15
1	A	174	PHE	CA-C-O	-5.77	113.92	120.32
1	A	166	ILE	CA-C-N	-5.76	112.78	122.29
1	A	166	ILE	C-N-CA	-5.76	112.78	122.29
1	A	174	PHE	CA-C-N	-5.75	114.59	122.93
1	A	174	PHE	C-N-CA	-5.75	114.59	122.93
1	A	339	LYS	CB-CA-C	-5.72	99.08	109.38
1	A	354	LYS	CA-C-O	-5.71	114.65	120.71
1	A	298	ARG	N-CA-C	-5.65	104.61	113.02
1	A	408	GLU	CA-C-N	5.64	124.99	118.85
1	A	408	GLU	C-N-CA	5.64	124.99	118.85
1	A	415	ASP	OD1-CG-OD2	5.63	136.41	122.90
1	A	271	GLU	CA-C-O	-5.61	114.47	120.92
1	A	423	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	A	432	GLU	CA-C-O	5.61	126.65	120.71
1	A	253	ARG	CG-CD-NE	5.59	124.29	112.00
1	A	323	ARG	CB-CA-C	5.56	119.86	110.79
1	A	414	SER	O-C-N	-5.54	115.02	122.94
1	A	211	GLU	CA-C-N	-5.53	113.19	122.92
1	A	211	GLU	C-N-CA	-5.53	113.19	122.92
1	A	283	ILE	CA-C-O	-5.50	115.31	121.36
1	A	268	PRO	O-C-N	-5.50	116.30	123.00
1	A	172	GLU	N-CA-CB	-5.49	101.31	111.53
1	A	414	SER	CA-C-O	5.47	128.13	121.68
1	A	164	GLU	N-CA-C	5.45	120.21	113.50
1	A	211	GLU	OE1-CD-OE2	5.45	135.99	122.90
1	A	405	LYS	CA-C-O	-5.44	114.39	120.54
1	A	317	ALA	CB-CA-C	-5.44	100.23	110.51
1	A	172	GLU	N-CA-C	5.44	117.66	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLN	CA-CB-CG	5.43	124.96	114.10
1	A	246	CYS	CB-CA-C	-5.42	100.99	109.72
1	A	326	THR	CA-C-N	5.42	125.72	119.92
1	A	326	THR	C-N-CA	5.42	125.72	119.92
1	A	275	MET	O-C-N	-5.41	117.58	123.26
1	A	279	THR	N-CA-CB	-5.40	101.55	111.37
1	A	375	THR	O-C-N	5.37	129.27	123.10
1	A	403	TYR	CA-C-O	-5.35	115.21	121.10
1	A	278	ARG	CA-C-O	5.35	126.81	120.66
1	A	412	ASN	CB-CG-ND2	-5.35	108.38	116.40
1	A	168	TYR	O-C-N	-5.35	116.86	123.33
1	A	273	GLU	O-C-N	-5.34	115.88	122.82
1	A	255	SER	N-CA-CB	-5.33	101.43	110.50
1	A	388	MET	CB-CA-C	-5.33	100.22	110.24
1	A	247	THR	CA-CB-OG1	-5.32	101.63	109.60
1	A	432	GLU	N-CA-C	5.32	118.15	109.59
1	A	264	SER	CA-C-N	-5.29	112.75	121.80
1	A	264	SER	C-N-CA	-5.29	112.75	121.80
1	A	430	ILE	CA-CB-CG1	-5.28	101.42	110.40
1	A	426	GLY	N-CA-C	-5.28	101.77	110.95
1	A	218	ASP	O-C-N	-5.27	115.58	122.59
1	A	287	PHE	CA-C-N	-5.27	115.56	122.99
1	A	287	PHE	C-N-CA	-5.27	115.56	122.99
1	A	197	SER	CB-CA-C	-5.25	100.10	109.71
1	A	285	LEU	CA-C-O	-5.24	114.30	119.49
1	A	422	VAL	CB-CA-C	-5.24	101.33	110.71
1	A	276	ARG	O-C-N	-5.24	116.88	123.27
1	A	199	ARG	NE-CZ-NH2	-5.24	114.49	119.20
1	A	334	GLN	O-C-N	-5.22	117.13	123.29
1	A	179	GLU	CA-C-N	-5.22	115.75	123.05
1	A	179	GLU	C-N-CA	-5.22	115.75	123.05
1	A	358	MET	CG-SD-CE	-5.21	89.44	100.90
1	A	317	ALA	N-CA-CB	5.19	118.31	110.42
1	A	400	LYS	CG-CD-CE	-5.18	99.39	111.30
1	A	430	ILE	CB-CA-C	-5.18	104.67	111.25
1	A	189	GLY	CA-C-N	5.17	129.97	121.39
1	A	189	GLY	C-N-CA	5.17	129.97	121.39
1	A	191	VAL	CA-CB-CG2	5.17	119.19	110.40
1	A	321	GLU	CG-CD-OE2	-5.16	106.52	118.40
1	A	180	SER	CA-C-N	-5.14	116.33	122.90
1	A	180	SER	C-N-CA	-5.14	116.33	122.90
1	A	382	ALA	CA-C-O	-5.14	115.58	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	CYS	CB-CA-C	5.14	119.86	110.10
1	A	390	PHE	CA-CB-CG	-5.12	108.67	113.80
1	A	163	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	A	374	PRO	CA-C-N	-5.11	113.49	121.87
1	A	374	PRO	C-N-CA	-5.11	113.49	121.87
2	P	2	TYR	CA-CB-CG	-5.10	104.72	113.90
1	A	408	GLU	OE1-CD-OE2	5.06	135.04	122.90
2	P	1	PHE	O-C-N	-5.05	114.92	123.00
1	A	206	LEU	CA-C-O	-5.04	115.25	120.70
1	A	254	LEU	CA-C-O	5.04	127.72	120.51
1	A	353	TRP	O-C-N	5.04	129.22	123.27
1	A	429	GLY	N-CA-C	-5.04	101.23	113.18
1	A	389	ASN	CA-C-N	-5.03	112.74	122.09
1	A	389	ASN	C-N-CA	-5.03	112.74	122.09
1	A	318	GLN	CB-CG-CD	-5.02	104.06	112.60

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	2159	83	0
2	P	56	0	58	6	0
3	A	44	0	0	3	1
3	P	3	0	0	1	0
All	All	2169	0	2217	85	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 20.

All (85) 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:280:THR:H	1:A:281:LYS:HZ2	1.10	0.99
1:A:220:ILE:HG12	1:A:242:ALA:HA	1.52	0.90
1:A:185:MET:HE1	1:A:288:ARG:HD2	1.58	0.84
1:A:281:LYS:H	1:A:281:LYS:NZ	1.81	0.77
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:HD12	1:A:328:LEU:N	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:376:ASN:HD22	1:A:376:ASN:C	2.01	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:H	1:A:328:LEU:CD1	2.05	0.66
1:A:238:LYS:HE2	1:A:239:GLN:HE21	1.62	0.64
1:A:281:LYS:H	1:A:281:LYS:HZ3	1.43	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:311:PHE:O	1:A:312:LYS:C	2.41	0.60
1:A:185:MET:HE2	3:A:5:HOH:O	2.02	0.60
1:A:207:SER:HB2	1:A:413:TYR:CE2	2.37	0.60
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: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:185:MET:CE	1:A:288:ARG:HD2	2.33	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:280:THR:H	1:A:281:LYS:NZ	1.95	0.55
1:A:169:ARG:CD	1:A:169:ARG:H	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:A:219:LYS:HA	1.90	0.53
1:A:414:SER:O	1:A:415:ASP:C	2.52	0.53
1:A:331:SER:HB3	1:A:373:LEU:HG	1.92	0.52
1:A:252:VAL:CG1	1:A:263:ILE:HG23	2.37	0.52
1:A:399:LEU:HD23	1:A:400:LYS:N	2.24	0.52
1:A:186:SER:HB2	1:A:187:PRO:CD	2.41	0.51
1:A:404:LEU:C	1:A:404:LEU:HD23	2.35	0.51
1:A:376:ASN:C	1:A:376:ASN:ND2	2.68	0.49
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:403:TYR:CD1	1:A:405:LYS:HG3	2.48	0.48
1:A:263:ILE:HD12	1:A:263:ILE:N	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:H	1:A:169:ARG:HD2	1.79	0.46
1:A:323:ARG:HH11	1:A:323:ARG:HD2	1.45	0.46
1:A:279:THR:HG21	1:A:397:SER:HB2	1.97	0.46
1:A:323:ARG:HH22	1:A:348:GLU:HB3	1.79	0.46
1:A:253:ARG:HD3	1:A:253:ARG:HA	1.44	0.45
1:A:311:PHE:O	1:A:360:GLY:HA3	2.17	0.45
1:A:159:ILE:HD13	1:A:209:MET:HE3	1.99	0.44
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: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
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:216:MET:HE3	1:A:218:ASP:HB2	2.01	0.41
1:A:210:PRO:O	1:A:266:ILE:HA	2.20	0.41
1:A:238:LYS:CE	1:A:239:GLN:HE21	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:HB2	1:A:402:ARG:NH2	2.28	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:403:TYR:CD1	1:A:403:TYR:C	2.98	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 ⓘ

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	250/314 (80%)	233 (93%)	14 (6%)	3 (1%)	10	20
2	P	4/6 (67%)	4 (100%)	0	0	100	100
All	All	254/320 (79%)	237 (93%)	14 (6%)	3 (1%)	10	20

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%)	213 (92%)	19 (8%)	10	23
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	237/287 (83%)	218 (92%)	19 (8%)	11	24

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	GLU
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	293	VAL
1	A	299	THR
1	A	328	LEU
1	A	339	LYS
1	A	341	LYS
1	A	343	LYS
1	A	377	ASP
1	A	396	PRO
1	A	408	GLU

Sometimes 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 oligosaccharides 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

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	256/314 (81%)	0.28	18 (7%)	22 20	46, 67, 105, 125	0
2	P	6/6 (100%)	1.28	2 (33%)	1 1	52, 70, 76, 87	0
All	All	262/320 (81%)	0.31	20 (7%)	20 17	46, 67, 103, 125	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	7.5
1	A	254	LEU	6.0
1	A	239	GLN	4.7
1	A	407	PHE	4.5
1	A	219	LYS	4.3
1	A	261	ARG	4.2
1	A	380	LYS	3.5
2	P	6	MET	3.4
1	A	379	LYS	3.1
1	A	169	ARG	3.1
2	P	1	PHE	2.9
1	A	262	SER	2.8
1	A	255	SER	2.7
1	A	260	GLU	2.7
1	A	377	ASP	2.4
1	A	161	TRP	2.4
1	A	211	GLU	2.3
1	A	376	ASN	2.2
1	A	238	LYS	2.1
1	A	281	LYS	2.1

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 oligosaccharides 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.