



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:30 AM UTC

PDB ID : 1Z9O / pdb_00001z9o
Title : 1.9 Angstrom Crystal Structure of the Rat VAP-A MSP Homology Domain in Complex with the Rat ORP1 FFAT Motif
Authors : Kaiser, S.E.; Brickner, J.H.; Reilein, A.R.; Fenn, T.D.; Walter, P.; Brunger, A.T.
Deposited on : 2005-04-03
Resolution : 1.90 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

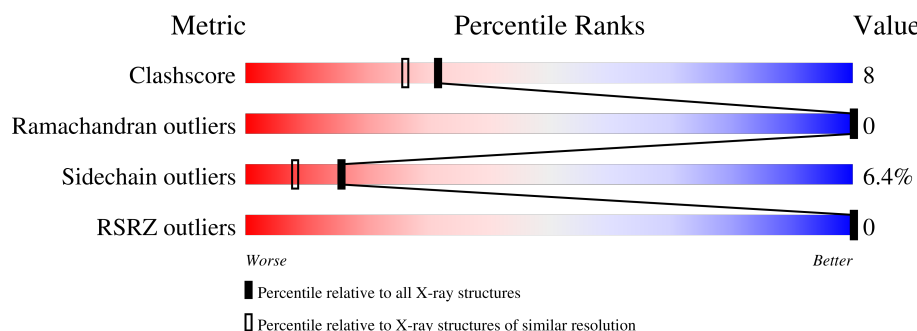
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



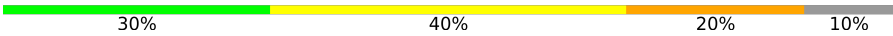
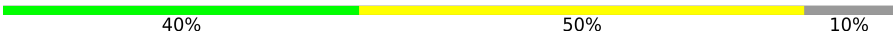
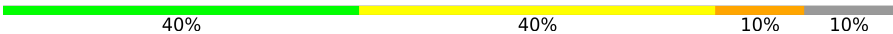
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	128	
1	B	128	
1	C	128	
1	D	128	
1	E	128	
1	F	128	

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Mol	Chain	Length	Quality of chain
2	G	10	
2	H	10	
2	I	10	
2	J	10	
2	K	10	
2	L	10	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6365 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 Vesicle-associated membrane protein-associated protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	1	0
			954	610	158	177	9			
1	B	119	Total	C	N	O	S	0	1	0
			954	610	158	177	9			
1	C	119	Total	C	N	O	S	0	1	0
			954	610	158	177	9			
1	D	119	Total	C	N	O	S	0	1	0
			954	610	158	177	9			
1	E	119	Total	C	N	O	S	0	1	0
			954	610	158	177	9			
1	F	119	Total	C	N	O	S	0	1	0
			954	610	158	177	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	GB 61889097
A	-1	SER	-	cloning artifact	GB 61889097
A	0	HIS	-	cloning artifact	GB 61889097
B	-2	GLY	-	cloning artifact	GB 61889097
B	-1	SER	-	cloning artifact	GB 61889097
B	0	HIS	-	cloning artifact	GB 61889097
C	-2	GLY	-	cloning artifact	GB 61889097
C	-1	SER	-	cloning artifact	GB 61889097
C	0	HIS	-	cloning artifact	GB 61889097
D	-2	GLY	-	cloning artifact	GB 61889097
D	-1	SER	-	cloning artifact	GB 61889097
D	0	HIS	-	cloning artifact	GB 61889097
E	-2	GLY	-	cloning artifact	GB 61889097
E	-1	SER	-	cloning artifact	GB 61889097
E	0	HIS	-	cloning artifact	GB 61889097
F	-2	GLY	-	cloning artifact	GB 61889097
F	-1	SER	-	cloning artifact	GB 61889097

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	cloning artifact	GB 61889097

- Molecule 2 is a protein called Oxysterol binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	14	0	0
			76	48	9	19			
2	H	9	Total	C	N	O	14	0	0
			76	48	9	19			
2	I	9	Total	C	N	O	14	0	0
			76	48	9	19			
2	J	9	Total	C	N	O	14	0	0
			76	48	9	19			
2	K	9	Total	C	N	O	14	0	0
			76	48	9	19			
2	L	9	Total	C	N	O	14	0	0
			76	48	9	19			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	32	Total	O	0	0
			32	32		
3	C	29	Total	O	0	0
			29	29		
3	D	24	Total	O	0	0
			24	24		
3	E	28	Total	O	0	0
			28	28		
3	F	31	Total	O	0	0
			31	31		
3	G	3	Total	O	0	0
			3	3		
3	H	1	Total	O	0	0
			1	1		
3	I	2	Total	O	0	0
			2	2		
3	J	2	Total	O	0	0
			2	2		
3	K	3	Total	O	0	0
			3	3		

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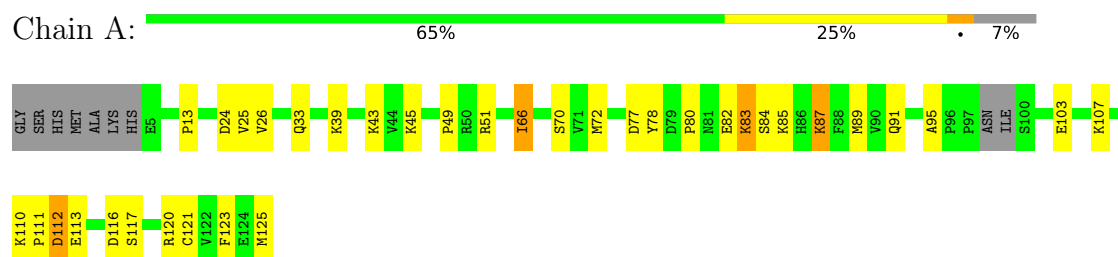
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	O	0	0
			1	1		

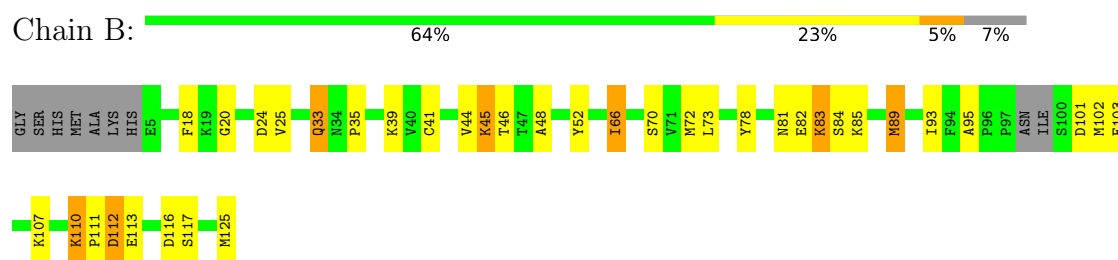
3 Residue-property plots [i](#)

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.

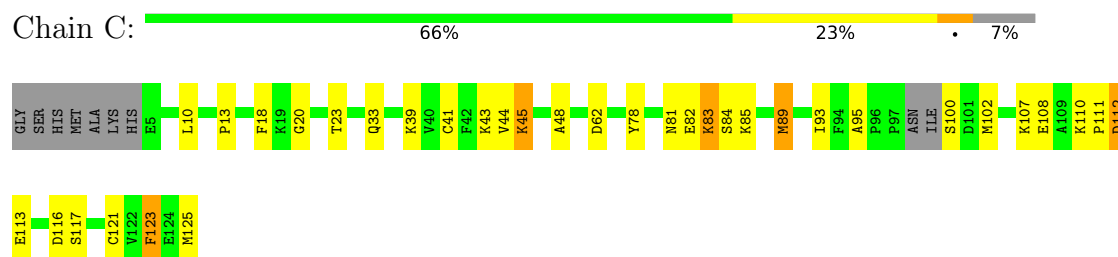
- Molecule 1: Vesicle-associated membrane protein-associated protein A



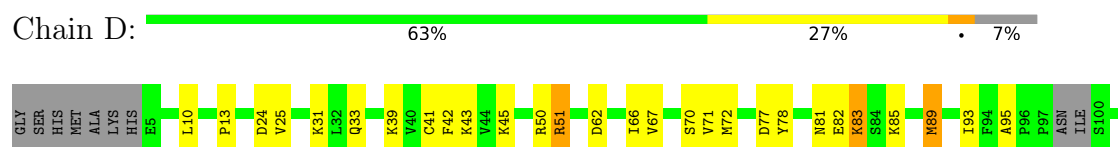
- Molecule 1: Vesicle-associated membrane protein-associated protein A



- Molecule 1: Vesicle-associated membrane protein-associated protein A



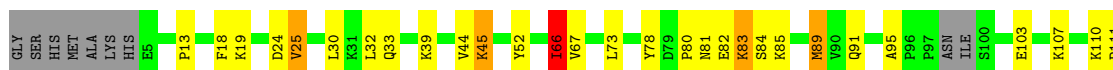
- Molecule 1: Vesicle-associated membrane protein-associated protein A





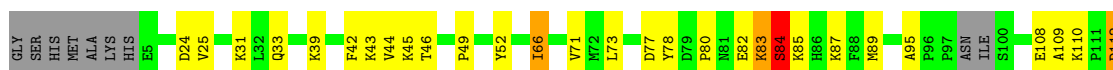
- Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain E: 63% 24% 5% 7%



- Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain F: 66% 23% 7%



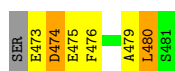
- Molecule 2: Oxysterol binding protein

Chain G: 40% 40% 10% 10%



- Molecule 2: Oxysterol binding protein

Chain H: 30% 40% 20% 10%



- Molecule 2: Oxysterol binding protein

Chain I: 50% 20% 20% 10%



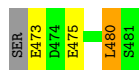
- Molecule 2: Oxysterol binding protein

Chain J: 40% 50% 10%



- Molecule 2: Oxysterol binding protein

Chain K:  60% 20% 10% 10%



- Molecule 2: Oxysterol binding protein

Chain L:  40% 40% 10% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.05Å 50.03Å 90.29Å 90.01° 90.00° 60.03°	Depositor
Resolution (Å)	14.65 – 1.90 14.65 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.65-1.90) 98.8 (14.65-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.74 (at 2.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.261 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.019 for k,-h+k,l 0.019 for h-k,h,l 0.467 for -h+k,-h,l 0.467 for -k,h-k,l 0.467 for -h+k,k,-l 0.477 for h,h-k,-l 0.019 for -h,-k,l 0.467 for -k,-h,-l 0.020 for k,h,-l 0.019 for h-k,-k,-l 0.019 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6365	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.20% 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	1.67	11/976 (1.1%)	1.41	4/1321 (0.3%)
1	B	1.71	10/976 (1.0%)	1.46	9/1321 (0.7%)
1	C	1.71	13/976 (1.3%)	1.44	9/1321 (0.7%)
1	D	1.69	10/976 (1.0%)	1.43	7/1321 (0.5%)
1	E	1.76	16/976 (1.6%)	1.43	5/1321 (0.4%)
1	F	1.72	13/976 (1.3%)	1.43	4/1321 (0.3%)
2	G	2.61	3/77 (3.9%)	1.59	1/103 (1.0%)
2	H	3.17	6/77 (7.8%)	1.66	2/103 (1.9%)
2	I	2.87	3/77 (3.9%)	1.59	0/103
2	J	2.91	4/77 (5.2%)	1.52	1/103 (1.0%)
2	K	2.60	2/77 (2.6%)	1.49	1/103 (1.0%)
2	L	2.57	4/77 (5.2%)	1.39	1/103 (1.0%)
All	All	1.81	95/6318 (1.5%)	1.44	44/8544 (0.5%)

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	F	0	1

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	473	GLU	CA-CB	-17.75	1.18	1.53
2	J	473	GLU	CA-CB	-14.46	1.24	1.53
2	K	473	GLU	CA-CB	-12.86	1.27	1.53
2	G	473	GLU	CA-CB	-11.75	1.29	1.53
2	I	474	ASP	CA-CB	-11.63	1.35	1.53
2	J	474	ASP	CA-CB	-11.37	1.36	1.53
2	G	475	GLU	CA-CB	-10.53	1.39	1.53
2	L	473	GLU	CA-CB	-9.89	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	475	GLU	CA-CB	-9.82	1.40	1.53
2	I	473	GLU	CA-CB	-9.64	1.34	1.53
1	E	89	MET	N-CA	-9.32	1.34	1.46
2	I	475	GLU	CA-CB	-9.24	1.41	1.53
2	H	475	GLU	CA-CB	-9.01	1.41	1.53
1	C	81	ASN	CG-OD1	8.86	1.40	1.23
1	E	44	VAL	CA-C	8.51	1.62	1.52
2	L	475	GLU	CA-CB	-8.24	1.42	1.53
1	F	45	LYS	CA-C	8.00	1.62	1.52
1	E	25	VAL	CA-CB	7.69	1.62	1.54
2	J	475	GLU	CA-CB	-7.55	1.43	1.53
2	H	474	ASP	CA-CB	-7.49	1.42	1.53
1	C	89	MET	N-CA	-7.44	1.36	1.46
1	B	45	LYS	CA-C	7.26	1.61	1.52
1	F	89	MET	N-CA	-7.20	1.37	1.46
1	C	45	LYS	CA-C	7.04	1.61	1.52
1	F	116	ASP	CB-CG	-6.82	1.35	1.52
1	A	89	MET	N-CA	-6.81	1.37	1.46
1	F	42	PHE	N-CA	6.71	1.54	1.45
2	L	480	LEU	C-O	-6.70	1.16	1.23
1	B	44	VAL	CA-CB	-6.68	1.46	1.54
1	F	71	VAL	CA-CB	6.66	1.62	1.53
1	B	116	ASP	N-CA	6.64	1.54	1.45
1	C	121	CYS	C-O	6.58	1.31	1.23
1	C	117	SER	N-CA	-6.39	1.38	1.45
1	E	32	LEU	C-O	6.39	1.31	1.24
1	B	89	MET	N-CA	-6.38	1.38	1.46
1	B	48	ALA	N-CA	6.35	1.53	1.46
1	C	116	ASP	CA-C	-6.34	1.44	1.52
1	E	116	ASP	CA-C	-6.33	1.44	1.52
2	G	474	ASP	CA-CB	-6.29	1.44	1.53
1	A	45	LYS	CA-C	6.20	1.60	1.52
2	L	474	ASP	CA-CB	-6.13	1.43	1.53
1	E	81	ASN	CG-ND2	6.12	1.46	1.33
1	C	116	ASP	N-CA	6.10	1.53	1.46
1	E	66	ILE	CA-C	6.10	1.60	1.52
1	A	91	GLN	CA-C	-6.01	1.45	1.52
1	D	89	MET	N-CA	-5.99	1.38	1.46
1	E	116	ASP	CB-CG	-5.99	1.37	1.52
1	D	123	PHE	CA-C	5.87	1.60	1.52
1	C	44	VAL	CA-C	5.85	1.59	1.52
1	F	31	LYS	C-O	5.81	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	ASN	CG-ND2	5.81	1.45	1.33
1	B	116	ASP	CA-C	-5.75	1.45	1.52
1	D	116	ASP	CB-CG	-5.74	1.37	1.52
1	E	124	GLU	N-CA	5.70	1.52	1.45
1	D	42	PHE	CA-C	5.69	1.59	1.52
1	F	123	PHE	CA-C	5.65	1.59	1.52
1	B	81	ASN	CG-ND2	5.58	1.45	1.33
1	D	116	ASP	N-CA	5.56	1.52	1.46
1	E	117	SER	C-O	-5.52	1.16	1.23
2	J	479	ALA	CA-CB	-5.51	1.44	1.53
1	D	31	LYS	C-O	5.50	1.30	1.24
1	A	13	PRO	CA-C	5.49	1.61	1.52
1	E	30	LEU	N-CA	-5.48	1.39	1.46
1	D	13	PRO	CA-C	5.45	1.61	1.52
1	B	117	SER	C-O	-5.45	1.16	1.23
1	A	116	ASP	CB-CG	-5.44	1.38	1.52
1	A	121	CYS	C-O	5.43	1.30	1.23
1	C	48	ALA	C-O	-5.42	1.17	1.23
1	A	26	VAL	C-O	-5.41	1.18	1.24
1	F	84	SER	N-CA	5.37	1.52	1.46
1	B	48	ALA	CA-CB	5.35	1.59	1.53
1	C	116	ASP	CB-CG	-5.35	1.38	1.52
1	F	46	THR	CA-C	-5.34	1.46	1.52
1	F	66	ILE	CA-C	5.30	1.59	1.52
1	B	116	ASP	CB-CG	-5.27	1.38	1.52
1	E	45	LYS	CA-C	5.24	1.59	1.52
1	F	44	VAL	CA-C	5.22	1.58	1.52
1	E	13	PRO	CA-C	5.20	1.60	1.52
1	A	116	ASP	CA-C	-5.19	1.46	1.52
1	C	123	PHE	CA-C	5.19	1.59	1.52
1	D	118	LYS	C-O	5.19	1.30	1.24
1	F	43	LYS	C-O	5.18	1.30	1.23
1	A	117	SER	C-O	-5.15	1.17	1.24
2	H	476	PHE	CA-C	5.15	1.59	1.52
1	A	116	ASP	N-CA	5.13	1.52	1.46
1	E	121	CYS	C-O	5.13	1.30	1.23
1	C	13	PRO	CA-C	5.09	1.59	1.52
1	A	66	ILE	CA-C	5.08	1.58	1.52
2	H	479	ALA	CA-CB	-5.07	1.44	1.53
1	D	71	VAL	CA-CB	5.05	1.60	1.53
1	E	91	GLN	CA-C	-5.05	1.46	1.52
1	E	114	LEU	C-O	5.02	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	118	LYS	C-O	5.02	1.30	1.24
2	H	479	ALA	N-CA	5.02	1.52	1.45
1	D	124	GLU	N-CA	5.01	1.51	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	473	GLU	CB-CA-C	9.86	128.84	110.10
1	D	116	ASP	CB-CA-C	-7.94	93.62	109.35
1	D	81	ASN	N-CA-C	7.66	122.47	113.20
1	C	81	ASN	OD1-CG-ND2	7.63	130.23	122.60
1	E	116	ASP	CB-CA-C	-7.45	94.59	109.35
2	J	473	GLU	CB-CA-C	7.06	123.51	110.10
1	D	82	GLU	CA-C-N	-6.95	111.81	122.09
1	D	82	GLU	C-N-CA	-6.95	111.81	122.09
1	A	116	ASP	CB-CA-C	-6.76	95.96	109.35
1	E	82	GLU	CA-C-N	-6.67	112.22	122.09
1	E	82	GLU	C-N-CA	-6.67	112.22	122.09
1	C	18	PHE	N-CA-C	6.56	119.11	108.41
1	F	116	ASP	CB-CA-C	-6.51	96.46	109.35
1	C	116	ASP	CB-CA-C	-6.47	96.54	109.35
1	C	82	GLU	CA-C-N	-6.25	111.37	122.07
1	C	82	GLU	C-N-CA	-6.25	111.37	122.07
1	B	82	GLU	CA-C-N	-6.22	111.43	122.07
1	B	82	GLU	C-N-CA	-6.22	111.43	122.07
1	A	82	GLU	CA-C-N	-6.18	111.50	122.07
1	A	82	GLU	C-N-CA	-6.18	111.50	122.07
1	B	116	ASP	CB-CA-C	-6.13	96.58	109.38
1	B	20	GLY	N-CA-C	5.99	119.19	112.00
1	F	82	GLU	CA-C-N	-5.80	112.15	122.07
1	F	82	GLU	C-N-CA	-5.80	112.15	122.07
1	A	87	LYS	CD-CE-NZ	-5.61	93.95	111.90
1	C	62	ASP	CA-C-N	-5.60	114.19	119.90
1	C	62	ASP	C-N-CA	-5.60	114.19	119.90
2	K	473	GLU	CB-CA-C	5.54	120.62	110.10
2	G	473	GLU	CB-CA-C	5.54	120.62	110.10
1	B	110	LYS	CA-C-N	-5.53	113.98	119.56
1	B	110	LYS	C-N-CA	-5.53	113.98	119.56
1	C	20	GLY	N-CA-C	5.43	118.52	112.00
2	L	473	GLU	CB-CA-C	5.42	120.40	110.10
1	D	51	ARG	CG-CD-NE	-5.42	100.09	112.00
1	B	18	PHE	N-CA-C	5.42	117.24	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	473	GLU	CA-CB-CG	5.31	124.72	114.10
1	E	18	PHE	N-CA-C	5.22	116.90	108.34
1	D	62	ASP	CA-C-N	-5.22	114.38	119.76
1	D	62	ASP	C-N-CA	-5.22	114.38	119.76
1	B	102	MET	N-CA-C	5.19	117.84	111.82
1	B	46	THR	N-CA-C	5.14	117.06	108.99
1	C	23	THR	N-CA-C	-5.06	107.06	113.18
1	E	19	LYS	N-CA-C	5.02	116.49	108.41
1	F	109	ALA	N-CA-C	5.01	117.56	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	84	SER	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	954	0	964	19	0
1	B	954	0	964	19	0
1	C	954	0	964	16	0
1	D	954	0	964	14	0
1	E	954	0	964	18	0
1	F	954	0	964	13	0
2	G	76	0	58	2	0
2	H	76	0	58	2	0
2	I	76	0	58	4	0
2	J	76	0	58	0	0
2	K	76	0	58	1	0
2	L	76	0	58	1	0
3	A	29	0	0	3	0
3	B	32	0	0	0	0
3	C	29	0	0	3	0
3	D	24	0	0	2	0
3	E	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	31	0	0	0	0
3	G	3	0	0	2	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	3	0	0	0	0
3	L	1	0	0	0	0
All	All	6365	0	6132	99	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 8.

All (99) 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:C:108:GLU:OE2	3:C:148:HOH:O	2.05	0.75
1:C:102:MET:HE3	3:C:138:HOH:O	1.88	0.73
3:G:148:HOH:O	2:I:480:LEU:HD11	1.88	0.73
1:F:112:ASP:OD1	1:F:112:ASP:N	2.24	0.70
1:E:78:TYR:CD2	1:E:125:MET:HE2	2.29	0.68
1:A:112:ASP:OD1	1:A:112:ASP:N	2.23	0.67
1:A:107:LYS:O	1:C:111:PRO:HB3	1.96	0.66
1:C:78:TYR:CD2	1:C:125:MET:HE2	2.31	0.66
1:B:112:ASP:OD1	1:B:112:ASP:N	2.31	0.64
1:A:111:PRO:HB3	1:C:107:LYS:O	1.98	0.64
1:B:111:PRO:HB3	1:E:107:LYS:O	2.01	0.60
1:C:112:ASP:OD1	1:C:112:ASP:N	2.29	0.60
1:A:51:ARG:CZ	3:A:146:HOH:O	2.49	0.60
1:D:24:ASP:OD2	1:D:25:VAL:N	2.32	0.60
1:A:110:LYS:HB2	1:A:113:GLU:HG3	1.84	0.60
1:C:102:MET:CE	3:C:138:HOH:O	2.49	0.60
1:E:24:ASP:OD2	1:E:25:VAL:N	2.34	0.59
1:C:110:LYS:HB2	1:C:113:GLU:HG3	1.86	0.58
1:F:110:LYS:HB2	1:F:113:GLU:HG3	1.86	0.57
1:C:39:LYS:HB2	1:C:95:ALA:HB3	1.86	0.57
1:B:24:ASP:OD2	1:B:25:VAL:N	2.36	0.57
1:B:110:LYS:HB2	1:B:113:GLU:HG3	1.87	0.57
1:D:112:ASP:OD1	1:D:112:ASP:N	2.33	0.55
1:A:103:GLU:HG3	2:I:474:ASP:O	2.07	0.54
1:C:45:LYS:HD3	1:C:89:MET:CE	2.37	0.54
1:E:112:ASP:OD1	1:E:112:ASP:N	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LYS:HB2	1:D:95:ALA:HB3	1.90	0.53
1:B:78:TYR:CD2	1:B:125:MET:HE2	2.43	0.53
1:B:83:LYS:HZ3	1:B:84:SER:H	1.58	0.52
1:D:45:LYS:HD3	1:D:89:MET:CE	2.40	0.51
1:E:45:LYS:HD3	1:E:89:MET:CE	2.41	0.51
1:B:45:LYS:HD3	1:B:89:MET:CE	2.41	0.51
1:D:70:SER:OG	1:D:72:MET:HE2	2.11	0.51
1:A:78:TYR:CD2	1:A:125:MET:HE2	2.46	0.51
1:B:107:LYS:O	1:E:111:PRO:HB3	2.11	0.51
1:A:24:ASP:OD2	1:A:25:VAL:N	2.44	0.51
1:D:50:ARG:HH11	1:D:50:ARG:HG2	1.75	0.50
1:F:24:ASP:OD2	1:F:25:VAL:N	2.45	0.49
1:B:39:LYS:HB2	1:B:95:ALA:HB3	1.93	0.49
1:D:51:ARG:CZ	3:D:134:HOH:O	2.60	0.49
1:A:49:PRO:HG3	2:G:477:TYR:HB2	1.95	0.49
3:G:148:HOH:O	2:I:480:LEU:CD1	2.54	0.49
1:B:45:LYS:HD3	1:B:89:MET:HE3	1.93	0.49
1:C:83:LYS:HZ3	1:C:84:SER:H	1.60	0.49
1:E:110:LYS:HB2	1:E:113:GLU:HG3	1.96	0.48
2:H:480:LEU:HD21	2:K:480:LEU:HD21	1.96	0.48
1:B:70:SER:OG	1:B:72:MET:HE2	2.14	0.48
1:B:41:CYS:HB2	1:B:93:ILE:HG22	1.96	0.48
1:C:83:LYS:HD2	1:C:83:LYS:HA	1.75	0.48
1:A:51:ARG:NH2	3:A:146:HOH:O	2.48	0.47
1:A:39:LYS:HB2	1:A:95:ALA:HB3	1.96	0.46
1:D:120:ARG:HG3	3:D:148:HOH:O	2.15	0.46
1:F:39:LYS:HB2	1:F:95:ALA:HB3	1.96	0.46
1:F:87:LYS:HZ2	1:F:87:LYS:HG2	1.51	0.46
1:E:83:LYS:HZ1	1:E:122:VAL:HA	1.81	0.46
1:A:83:LYS:HE3	1:A:123:PHE:HB2	1.98	0.46
2:G:480:LEU:HD21	2:I:480:LEU:HD21	1.97	0.45
1:A:70:SER:OG	1:A:72:MET:HE2	2.17	0.45
1:A:83:LYS:HA	1:A:83:LYS:HD2	1.47	0.44
1:D:78:TYR:CD2	1:D:125:MET:HE2	2.52	0.44
1:F:78:TYR:CD2	1:F:125:MET:HE2	2.52	0.44
1:E:83:LYS:HE2	1:E:84:SER:H	1.83	0.44
1:A:83:LYS:CE	1:A:84:SER:H	2.31	0.44
1:B:83:LYS:NZ	1:B:84:SER:H	2.16	0.43
1:F:49:PRO:HG3	2:L:477:TYR:HB2	1.99	0.43
1:E:78:TYR:CZ	1:E:80:PRO:HA	2.52	0.43
1:C:41:CYS:HB2	1:C:93:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:O	1:B:35:PRO:HD3	2.19	0.43
1:B:33:GLN:HB2	1:B:66:ILE:HD12	2.01	0.43
1:B:101:ASP:OD2	1:B:103:GLU:HB2	2.19	0.43
1:B:52:TYR:CE1	1:B:73:LEU:HD13	2.54	0.42
1:E:39:LYS:HB2	1:E:95:ALA:HB3	2.00	0.42
1:F:83:LYS:CE	1:F:84:SER:H	2.32	0.42
1:A:87:LYS:HZ2	1:A:87:LYS:HG2	1.40	0.42
1:F:83:LYS:HE3	1:F:123:PHE:HB2	2.02	0.42
1:E:83:LYS:HD2	1:E:83:LYS:HA	1.82	0.42
1:D:110:LYS:HB2	1:D:113:GLU:HG3	2.01	0.42
1:F:114:LEU:HD23	1:F:114:LEU:HA	1.86	0.42
1:A:83:LYS:HZ3	1:A:83:LYS:HG3	1.45	0.41
1:D:45:LYS:HD3	1:D:89:MET:HE3	2.01	0.41
1:D:83:LYS:HZ3	1:D:83:LYS:HG3	1.37	0.41
1:F:83:LYS:HA	1:F:83:LYS:HD2	1.44	0.41
1:A:120:ARG:HG3	3:A:137:HOH:O	2.20	0.41
1:E:83:LYS:CE	1:E:84:SER:H	2.34	0.41
1:E:103:GLU:HG3	2:H:474:ASP:O	2.20	0.41
1:B:83:LYS:CE	1:B:84:SER:H	2.33	0.41
1:C:83:LYS:HZ3	1:C:83:LYS:HG3	1.70	0.41
1:C:83:LYS:HZ1	1:C:123:PHE:H	1.68	0.41
1:C:83:LYS:CE	1:C:84:SER:H	2.33	0.41
1:D:41:CYS:HB2	1:D:93:ILE:HG22	2.02	0.41
1:D:67:VAL:O	1:D:67:VAL:HG23	2.21	0.41
1:E:52:TYR:CE1	1:E:73:LEU:HD13	2.56	0.41
1:F:78:TYR:CZ	1:F:80:PRO:HA	2.56	0.40
1:E:66:ILE:HG13	1:E:67:VAL:N	2.37	0.40
1:F:52:TYR:CE1	1:F:73:LEU:HD13	2.56	0.40
1:B:33:GLN:HE21	1:B:33:GLN:HB3	1.72	0.40
1:E:114:LEU:HA	1:E:114:LEU:HD23	1.79	0.40
1:A:78:TYR:CZ	1:A:80:PRO:HA	2.57	0.40
1:E:83:LYS:HZ3	1:E:83:LYS:HG3	1.79	0.40

There are no symmetry-related clashes.

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	116/128 (91%)	113 (97%)	3 (3%)	0	100	100
1	B	116/128 (91%)	114 (98%)	2 (2%)	0	100	100
1	C	116/128 (91%)	114 (98%)	2 (2%)	0	100	100
1	D	116/128 (91%)	113 (97%)	3 (3%)	0	100	100
1	E	116/128 (91%)	113 (97%)	3 (3%)	0	100	100
1	F	116/128 (91%)	113 (97%)	3 (3%)	0	100	100
2	G	7/10 (70%)	7 (100%)	0	0	100	100
2	H	7/10 (70%)	7 (100%)	0	0	100	100
2	I	7/10 (70%)	7 (100%)	0	0	100	100
2	J	7/10 (70%)	7 (100%)	0	0	100	100
2	K	7/10 (70%)	7 (100%)	0	0	100	100
2	L	7/10 (70%)	7 (100%)	0	0	100	100
All	All	738/828 (89%)	722 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	113/119 (95%)	106 (94%)	7 (6%)	16	9
1	B	113/119 (95%)	108 (96%)	5 (4%)	25	17
1	C	113/119 (95%)	106 (94%)	7 (6%)	16	9
1	D	113/119 (95%)	104 (92%)	9 (8%)	11	5
1	E	113/119 (95%)	108 (96%)	5 (4%)	25	17
1	F	113/119 (95%)	106 (94%)	7 (6%)	16	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	8/9 (89%)	7 (88%)	1 (12%)	4	1
2	H	8/9 (89%)	7 (88%)	1 (12%)	4	1
2	I	8/9 (89%)	7 (88%)	1 (12%)	4	1
2	J	8/9 (89%)	7 (88%)	1 (12%)	4	1
2	K	8/9 (89%)	7 (88%)	1 (12%)	4	1
2	L	8/9 (89%)	7 (88%)	1 (12%)	4	1
All	All	726/768 (94%)	680 (94%)	46 (6%)	16	8

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	43	LYS
1	A	66	ILE
1	A	77	ASP
1	A	83	LYS
1	A	85	LYS
1	A	112	ASP
1	B	33	GLN
1	B	66	ILE
1	B	83	LYS
1	B	85	LYS
1	B	112	ASP
1	C	10	LEU
1	C	33	GLN
1	C	43	LYS
1	C	83	LYS
1	C	85	LYS
1	C	100	SER
1	C	112	ASP
1	D	10	LEU
1	D	33	GLN
1	D	43	LYS
1	D	66	ILE
1	D	77	ASP
1	D	83	LYS
1	D	85	LYS
1	D	112	ASP
1	D	119	LEU
1	E	33	GLN

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Mol	Chain	Res	Type
1	E	66	ILE
1	E	83	LYS
1	E	85	LYS
1	E	112	ASP
1	F	33	GLN
1	F	66	ILE
1	F	77	ASP
1	F	83	LYS
1	F	85	LYS
1	F	108	GLU
1	F	112	ASP
2	G	480	LEU
2	H	480	LEU
2	I	480	LEU
2	J	480	LEU
2	K	480	LEU
2	L	480	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	33	GLN
1	B	29	ASN
1	B	33	GLN
1	B	91	GLN
1	C	33	GLN
1	C	91	GLN
1	D	33	GLN
1	E	33	GLN
1	F	33	GLN
1	F	91	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 [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 [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	119/128 (92%)	-1.28	0 100 100	13, 28, 33, 37	1 (0%)
1	B	119/128 (92%)	-1.31	0 100 100	13, 28, 37, 48	1 (0%)
1	C	119/128 (92%)	-1.36	0 100 100	13, 28, 36, 46	1 (0%)
1	D	119/128 (92%)	-1.31	0 100 100	13, 28, 35, 47	1 (0%)
1	E	119/128 (92%)	-1.35	0 100 100	13, 28, 37, 48	1 (0%)
1	F	119/128 (92%)	-1.31	0 100 100	13, 28, 33, 37	1 (0%)
2	G	9/10 (90%)	-1.41	0 100 100	11, 20, 28, 30	3 (33%)
2	H	9/10 (90%)	-1.30	0 100 100	11, 20, 30, 30	3 (33%)
2	I	9/10 (90%)	-1.42	0 100 100	12, 20, 30, 31	3 (33%)
2	J	9/10 (90%)	-1.40	0 100 100	11, 20, 30, 31	3 (33%)
2	K	9/10 (90%)	-1.38	0 100 100	11, 20, 30, 31	3 (33%)
2	L	9/10 (90%)	-1.35	0 100 100	11, 20, 28, 30	3 (33%)
All	All	768/828 (92%)	-1.33	0 100 100	11, 28, 35, 48	24 (3%)

There are no RSRZ outliers to report.

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.