Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 04:51 AM EDT

PDB ID	:	1Z9O
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 (i) 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 (1)) were used in the production of this report:

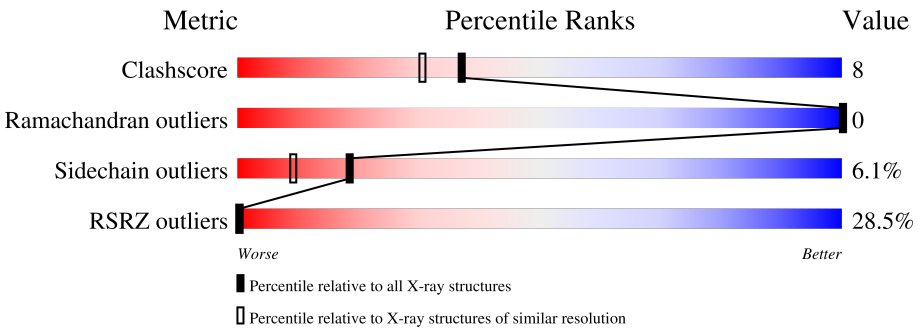
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	27% 69% 20% • 7%
1	B	128	28% 66% 23% • 7%
1	C	128	24% 71% 20% • 7%
1	D	128	30% 70% 20% • • 7%
1	E	128	27% 66% 22% 5% 7%
1	F	128	25% 70% 20% • 7%
2	G	10	50% 30% 10% 10%

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Mol	Chain	Length	Quality of chain
2	H	10	10% 50% 20% 20% 10%
2	I	10	30% 50% 20% 20% 10%
2	J	10	20% 60% 30% 10%
2	K	10	30% 60% 20% 10% 10%
2	L	10	30% 50% 40% 10%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	119	954	610	158	177	9	0	1	0
1	B	119	954	610	158	177	9	0	1	0
1	C	119	954	610	158	177	9	0	1	0
1	D	119	954	610	158	177	9	0	1	0
1	E	119	954	610	158	177	9	0	1	0
1	F	119	954	610	158	177	9	0	1	0

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
			Total	C	N	O			
2	G	9	76	48	9	19	14	0	0
2	H	9	76	48	9	19	14	0	0
2	I	9	76	48	9	19	14	0	0
2	J	9	76	48	9	19	14	0	0
2	K	9	76	48	9	19	14	0	0
2	L	9	76	48	9	19	14	0	0

- Molecule 3 is water.

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

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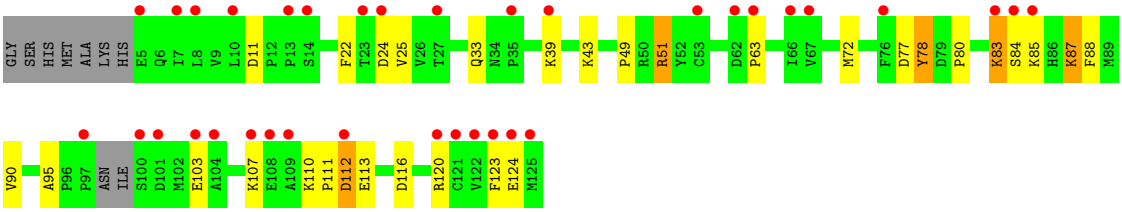
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	L	1	1	1	0	0

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.

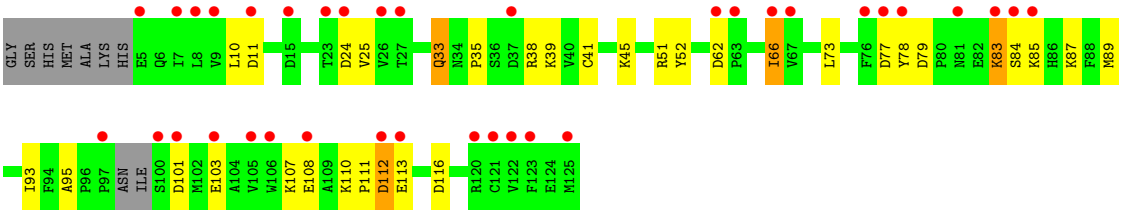
• Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain A:



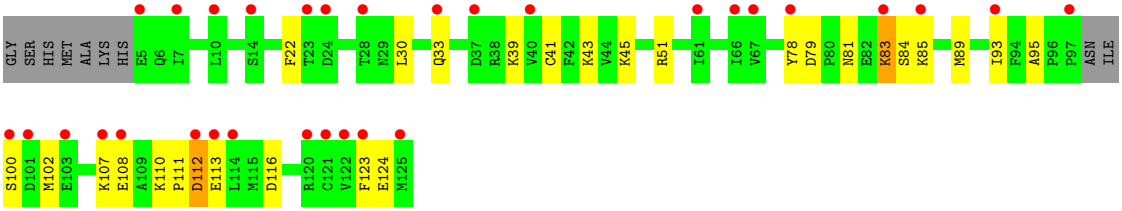
• Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain B:



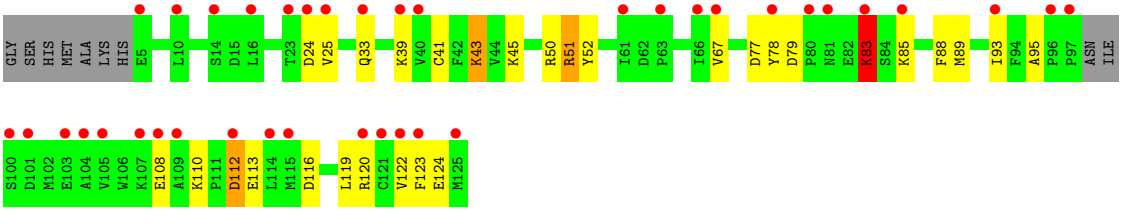
• Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain C:



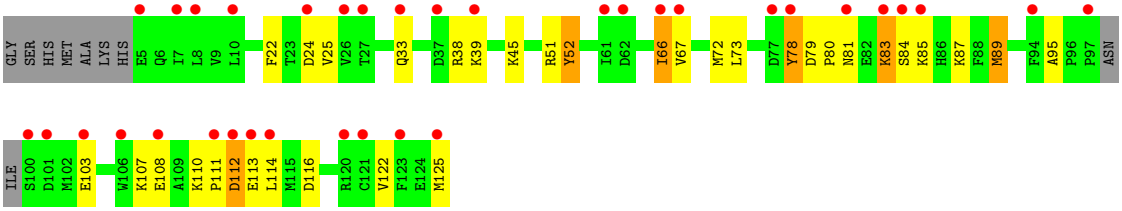
• Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain D:



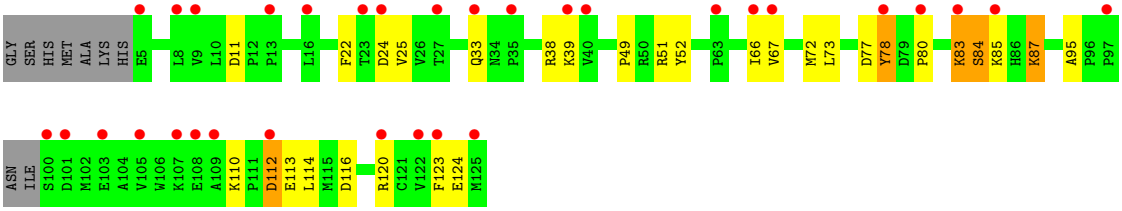
• Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain E:



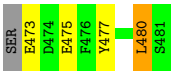
• Molecule 1: Vesicle-associated membrane protein-associated protein A

Chain F:



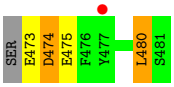
• Molecule 2: Oxysterol binding protein

Chain G:



• Molecule 2: Oxysterol binding protein

Chain H:

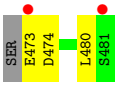


• Molecule 2: Oxysterol binding protein

Chain I:

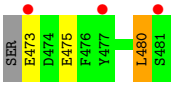
• Molecule 2: Oxysterol binding protein

Chain J:



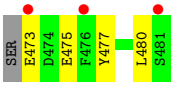
• Molecule 2: Oxysterol binding protein

Chain K:



• Molecule 2: Oxysterol binding protein

Chain L:



4 Data and refinement statistics (i)

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 17.59 – 2.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.65-1.90) 98.8 (17.59-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.74 (at 2.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.261 0.229 , (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)	0.31 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	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	0.90	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.41	8/976 (0.8%)	1.28	9/1321 (0.7%)
1	B	1.43	4/976 (0.4%)	1.30	10/1321 (0.8%)
1	C	1.42	7/976 (0.7%)	1.26	5/1321 (0.4%)
1	D	1.42	6/976 (0.6%)	1.24	8/1321 (0.6%)
1	E	1.43	7/976 (0.7%)	1.28	7/1321 (0.5%)
1	F	1.46	6/976 (0.6%)	1.33	11/1321 (0.8%)
2	G	2.17	2/77 (2.6%)	1.35	1/103 (1.0%)
2	H	2.69	3/77 (3.9%)	1.53	2/103 (1.9%)
2	I	2.33	3/77 (3.9%)	1.42	0/103
2	J	2.49	2/77 (2.6%)	1.43	1/103 (1.0%)
2	K	2.29	2/77 (2.6%)	1.40	1/103 (1.0%)
2	L	2.14	2/77 (2.6%)	1.31	0/103
All	All	1.52	52/6318 (0.8%)	1.29	55/8544 (0.6%)

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 (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	473	GLU	CA-CB	-16.36	1.18	1.53
2	J	473	GLU	CA-CB	-13.38	1.24	1.53
2	K	473	GLU	CA-CB	-11.92	1.27	1.53
2	G	473	GLU	CA-CB	-10.91	1.29	1.53
2	L	473	GLU	CA-CB	-9.22	1.33	1.53
2	I	473	GLU	CA-CB	-8.99	1.34	1.53
2	I	474	ASP	CA-CB	-8.51	1.35	1.53
1	F	116	ASP	CB-CG	-7.98	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	474	ASP	CA-CB	-7.82	1.36	1.53
1	C	81	ASN	CG-OD1	7.47	1.40	1.24
1	E	116	ASP	CB-CG	-6.99	1.37	1.51
2	G	475	GLU	CA-CB	-6.70	1.39	1.53
1	D	116	ASP	CB-CG	-6.69	1.37	1.51
1	F	124	GLU	CB-CG	6.60	1.64	1.52
1	F	22	PHE	CE1-CZ	6.52	1.49	1.37
1	C	124	GLU	CB-CG	6.39	1.64	1.52
1	D	124	GLU	CB-CG	6.36	1.64	1.52
1	A	116	ASP	CB-CG	-6.33	1.38	1.51
2	K	475	GLU	CA-CB	-6.27	1.40	1.53
1	C	116	ASP	CB-CG	-6.23	1.38	1.51
1	B	116	ASP	CB-CG	-6.13	1.38	1.51
1	B	78	TYR	CE2-CZ	6.08	1.46	1.38
1	F	67	VAL	CB-CG2	-6.02	1.40	1.52
1	E	89	MET	N-CA	-5.99	1.34	1.46
1	A	78	TYR	CE2-CZ	5.96	1.46	1.38
1	F	78	TYR	CE2-CZ	5.89	1.46	1.38
2	I	475	GLU	CA-CB	-5.81	1.41	1.53
1	A	124	GLU	CB-CG	5.81	1.63	1.52
1	A	78	TYR	CD2-CE2	5.78	1.48	1.39
2	H	475	GLU	CA-CB	-5.78	1.41	1.53
1	D	78	TYR	CE2-CZ	5.74	1.46	1.38
1	F	78	TYR	CD2-CE2	5.66	1.47	1.39
1	A	88	PHE	CG-CD2	-5.59	1.30	1.38
1	A	124	GLU	CG-CD	5.58	1.60	1.51
1	E	108	GLU	CG-CD	5.54	1.60	1.51
1	A	22	PHE	CE1-CZ	5.48	1.47	1.37
1	E	52	TYR	CD1-CE1	-5.46	1.31	1.39
1	B	108	GLU	CG-CD	5.42	1.60	1.51
1	C	78	TYR	CD2-CE2	5.36	1.47	1.39
2	L	475	GLU	CA-CB	-5.30	1.42	1.53
1	E	81	ASN	CG-ND2	5.30	1.46	1.32
2	H	474	ASP	CA-CB	-5.29	1.42	1.53
1	C	22	PHE	CE1-CZ	5.21	1.47	1.37
1	E	78	TYR	CE2-CZ	5.20	1.45	1.38
1	D	52	TYR	CE2-CZ	-5.14	1.31	1.38
1	E	22	PHE	CE1-CZ	5.10	1.47	1.37
1	D	88	PHE	CD2-CE2	5.09	1.49	1.39
1	D	43	LYS	CE-NZ	5.05	1.61	1.49
1	C	81	ASN	CG-ND2	5.04	1.45	1.32
1	C	78	TYR	CE2-CZ	5.03	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	VAL	CB-CG2	-5.02	1.42	1.52
1	B	78	TYR	CE1-CZ	-5.01	1.32	1.38

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	116	ASP	CB-CG-OD2	-12.45	107.10	118.30
1	E	116	ASP	CB-CG-OD2	-10.72	108.65	118.30
2	H	473	GLU	CB-CA-C	9.22	128.84	110.40
1	C	116	ASP	CB-CG-OD2	-9.15	110.06	118.30
1	D	116	ASP	CB-CA-C	-8.39	93.62	110.40
1	A	51	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	E	51	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	E	116	ASP	CB-CA-C	-7.91	94.59	110.40
1	A	87	LYS	CD-CE-NZ	-7.72	93.95	111.70
1	B	116	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	116	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	D	116	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	116	ASP	CB-CA-C	-7.22	95.96	110.40
1	F	51	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	51	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	F	116	ASP	CB-CA-C	-6.97	96.46	110.40
1	C	116	ASP	CB-CA-C	-6.93	96.54	110.40
1	B	116	ASP	CB-CA-C	-6.91	96.58	110.40
1	F	87	LYS	CD-CE-NZ	-6.69	96.32	111.70
1	D	51	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	D	79	ASP	CB-CG-OD1	6.64	124.28	118.30
2	J	473	GLU	CB-CA-C	6.55	123.51	110.40
1	C	51	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	87	LYS	CD-CE-NZ	-6.10	97.66	111.70
1	B	11	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	F	72	MET	CG-SD-CE	-5.99	90.62	100.20
1	B	38	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	F	11	ASP	CB-CG-OD1	-5.85	113.04	118.30
1	B	10	LEU	CB-CG-CD2	5.78	120.83	111.00
1	B	11	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	79	ASP	CB-CG-OD1	5.67	123.41	118.30
1	D	51	ARG	CG-CD-NE	-5.58	100.09	111.80
1	F	120	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	38	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	79	ASP	CB-CG-OD1	5.49	123.24	118.30
1	F	11	ASP	CB-CG-OD2	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	TYR	CZ-CE2-CD2	-5.45	114.89	119.80
1	F	116	ASP	OD1-CG-OD2	5.45	133.66	123.30
1	B	62	ASP	CB-CG-OD1	5.42	123.17	118.30
1	C	30	LEU	CB-CG-CD2	-5.36	101.88	111.00
1	C	79	ASP	CB-CG-OD1	5.33	123.10	118.30
1	F	51	ARG	CD-NE-CZ	5.30	131.02	123.60
1	D	78	TYR	CZ-CE2-CD2	-5.28	115.05	119.80
1	A	11	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	51	ARG	CD-NE-CZ	5.17	130.84	123.60
1	D	83	LYS	CD-CE-NZ	-5.16	99.84	111.70
2	H	473	GLU	CA-CB-CG	5.15	124.72	113.40
1	D	78	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	E	72	MET	CG-SD-CE	-5.12	92.01	100.20
2	G	473	GLU	CB-CA-C	5.11	120.62	110.40
2	K	473	GLU	CB-CA-C	5.11	120.62	110.40
1	E	87	LYS	CD-CE-NZ	-5.09	99.99	111.70
1	A	72	MET	CG-SD-CE	-5.05	92.11	100.20
1	F	38	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	78	TYR	CB-CG-CD1	-5.04	117.98	121.00

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 (i)

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	17	0
1	B	954	0	964	17	0
1	C	954	0	964	16	0
1	D	954	0	964	13	0
1	E	954	0	964	19	0
1	F	954	0	964	13	0
2	G	76	0	58	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	95	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 (95) 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
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: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:B:112:ASP:N	1:B:112:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:LYS:HZ3	1:B:84:SER:H	1.52	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
1:D:39:LYS:HB2	1:D:95:ALA:HB3	1.90	0.53
1:C:102:MET:HE2	3:C:138:HOH:O	2.06	0.53
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: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: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: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:D:83:LYS:HZ3	1:D:83:LYS:HG3	1.59	0.47
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:C:45:LYS:HD3	1:C:89:MET:HE3	1.98	0.45
1:A:83:LYS:HA	1:A:83:LYS:HD2	1.47	0.44
1:B:45:LYS:HD3	1:B:89:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:83:LYS:HZ3	1:F:83:LYS:HG3	1.64	0.43
1:C:41:CYS:HB2	1:C:93:ILE:HG22	2.01	0.43
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:83:LYS:HZ3	1:A:84:SER:H	1.67	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:E:78:TYR:CD2	1:E:125:MET:CE	3.03	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:D:83:LYS:HZ1	1:D:123:PHE:H	1.68	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:78:TYR:CD2	1:E:125:MET:HE1	2.55	0.41
1:E:52:TYR:CE1	1:E:73:LEU:HD13	2.56	0.41
1:A:87:LYS:HZ2	1:A:87:LYS:HG2	1.53	0.40
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:D:83:LYS:HZ1	1:D:122:VAL:HA	1.87	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 (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	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 (i)

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%)	18	9
1	B	113/119 (95%)	107 (95%)	6 (5%)	22	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	113/119 (95%)	107 (95%)	6 (5%)	22	13
1	D	113/119 (95%)	105 (93%)	8 (7%)	14	6
1	E	113/119 (95%)	108 (96%)	5 (4%)	28	19
1	F	113/119 (95%)	107 (95%)	6 (5%)	22	13
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%)	682 (94%)	44 (6%)	18	9

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	43	LYS
1	A	63	PRO
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	77	ASP
1	B	83	LYS
1	B	85	LYS
1	B	112	ASP
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	33	GLN
1	D	43	LYS
1	D	77	ASP
1	D	83	LYS

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Mol	Chain	Res	Type
1	D	85	LYS
1	D	108	GLU
1	D	112	ASP
1	D	119	LEU
1	E	33	GLN
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	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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	B	33	GLN
1	C	33	GLN
1	D	33	GLN
1	E	33	GLN
1	F	29	ASN
1	F	33	GLN

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 monosaccharides 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%)	1.54	35 (29%)	0	0	22, 28, 33, 37	0
1	B	119/128 (92%)	1.61	36 (30%)	0	0	21, 28, 37, 48	0
1	C	119/128 (92%)	1.54	31 (26%)	0	0	19, 28, 36, 46	0
1	D	119/128 (92%)	1.60	38 (31%)	0	0	21, 28, 35, 47	0
1	E	119/128 (92%)	1.60	35 (29%)	0	0	20, 28, 37, 48	0
1	F	119/128 (92%)	1.54	32 (26%)	0	0	22, 28, 33, 37	0
2	G	9/10 (90%)	1.13	0	100	100	20, 25, 33, 34	3 (33%)
2	H	9/10 (90%)	1.08	1 (11%)	5	6	20, 25, 34, 34	3 (33%)
2	I	9/10 (90%)	1.66	3 (33%)	0	0	20, 26, 33, 34	3 (33%)
2	J	9/10 (90%)	1.32	2 (22%)	0	0	20, 25, 34, 34	3 (33%)
2	K	9/10 (90%)	1.38	3 (33%)	0	0	20, 25, 34, 35	3 (33%)
2	L	9/10 (90%)	1.30	3 (33%)	0	0	20, 25, 33, 34	3 (33%)
All	All	768/828 (92%)	1.55	219 (28%)	0	0	19, 28, 35, 48	18 (2%)

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	85	LYS	4.9
1	E	103	GLU	4.8
1	A	101	ASP	4.8
1	F	101	ASP	4.6
1	C	123	PHE	4.3
1	C	112	ASP	4.3
1	E	123	PHE	4.2
1	D	66	ILE	4.2
1	C	120	ARG	4.2
1	C	85	LYS	4.1
1	E	112	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	97	PRO	4.1
1	B	123	PHE	4.1
1	F	97	PRO	4.1
1	E	5	GLU	4.0
1	F	83	LYS	4.0
1	B	7	ILE	4.0
1	A	123	PHE	4.0
1	D	112	ASP	4.0
1	E	101	ASP	4.0
2	I	473	GLU	4.0
1	E	66	ILE	3.9
1	D	101	ASP	3.9
1	B	101	ASP	3.9
1	B	125	MET	3.9
1	A	85	LYS	3.8
1	B	100	SER	3.8
1	A	63	PRO	3.8
1	B	103	GLU	3.8
1	B	120	ARG	3.8
1	D	125	MET	3.8
1	D	103	GLU	3.8
1	B	85	LYS	3.7
1	B	24	ASP	3.7
1	A	66	ILE	3.6
1	C	66	ILE	3.6
1	A	97	PRO	3.6
1	B	97	PRO	3.6
1	D	78	TYR	3.6
1	E	108	GLU	3.6
1	D	14	SER	3.6
1	C	101	ASP	3.6
1	D	97	PRO	3.6
1	F	120	ARG	3.6
1	E	7	ILE	3.5
1	F	66	ILE	3.5
1	F	103	GLU	3.5
1	F	122	VAL	3.5
1	B	5	GLU	3.4
1	C	5	GLU	3.4
1	F	123	PHE	3.4
1	A	7	ILE	3.4
1	B	66	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	120	ARG	3.3
1	F	125	MET	3.3
1	E	24	ASP	3.3
1	D	100	SER	3.3
1	D	5	GLU	3.2
1	E	125	MET	3.2
1	A	121	CYS	3.2
1	B	121	CYS	3.2
1	A	112	ASP	3.2
1	B	112	ASP	3.2
1	B	108	GLU	3.2
1	E	85	LYS	3.2
1	E	120	ARG	3.2
1	F	100	SER	3.1
1	D	123	PHE	3.1
1	A	100	SER	3.1
1	A	83	LYS	3.1
1	B	122	VAL	3.1
1	B	23	THR	3.0
2	I	474	ASP	3.0
1	D	83	LYS	3.0
2	I	481	SER	3.0
1	F	24	ASP	3.0
1	D	120	ARG	3.0
1	C	33	GLN	3.0
1	C	97	PRO	3.0
1	D	108	GLU	2.9
1	C	108	GLU	2.9
1	D	122	VAL	2.9
1	F	112	ASP	2.9
1	A	103	GLU	2.9
1	D	24	ASP	2.9
1	E	83	LYS	2.9
1	E	100	SER	2.9
1	C	103	GLU	2.8
1	B	67	VAL	2.8
1	C	114	LEU	2.8
1	A	24	ASP	2.8
2	J	473	GLU	2.8
1	C	61	ILE	2.8
1	C	125	MET	2.8
1	E	113	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	63	PRO	2.7
1	E	114	LEU	2.7
1	A	122	VAL	2.7
1	F	39	LYS	2.7
1	D	23	THR	2.7
1	F	9	VAL	2.7
1	B	83	LYS	2.7
1	A	23	THR	2.7
1	C	24	ASP	2.7
1	B	84	SER	2.7
1	C	67	VAL	2.6
1	B	81	ASN	2.6
1	B	8	LEU	2.6
1	A	5	GLU	2.6
1	A	67	VAL	2.6
1	B	9	VAL	2.6
1	C	28	THR	2.6
1	C	107	LYS	2.6
1	D	39	LYS	2.6
1	D	85	LYS	2.6
1	B	77	ASP	2.6
1	C	83	LYS	2.6
1	D	33	GLN	2.6
1	D	121	CYS	2.6
1	E	26	VAL	2.6
2	K	481	SER	2.5
1	C	122	VAL	2.5
1	D	109	ALA	2.5
1	A	10	LEU	2.5
1	E	37	ASP	2.5
1	E	27	THR	2.5
1	A	84	SER	2.5
1	F	105	VAL	2.5
1	B	62	ASP	2.5
1	C	37	ASP	2.5
1	A	62	ASP	2.5
1	E	61	ILE	2.5
1	B	63	PRO	2.5
1	D	25	VAL	2.5
1	A	14	SER	2.5
1	C	14	SER	2.5
2	J	481	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	104	ALA	2.5
1	B	105	VAL	2.5
1	E	33	GLN	2.5
1	D	114	LEU	2.5
1	B	15	ASP	2.4
1	C	78	TYR	2.4
1	E	81	ASN	2.4
1	D	107	LYS	2.4
1	F	107	LYS	2.4
1	E	10	LEU	2.4
1	A	107	LYS	2.4
1	E	39	LYS	2.4
1	F	5	GLU	2.4
1	F	35	PRO	2.4
1	B	106	TRP	2.4
1	E	77	ASP	2.4
1	A	13	PRO	2.4
1	D	80	PRO	2.4
1	A	39	LYS	2.4
2	K	473	GLU	2.4
1	A	125	MET	2.4
1	A	27	THR	2.4
1	A	104	ALA	2.3
1	F	23	THR	2.3
1	B	26	VAL	2.3
1	C	93	ILE	2.3
1	D	67	VAL	2.3
1	C	7	ILE	2.3
1	D	115	MET	2.3
1	D	63	PRO	2.3
1	D	40	VAL	2.3
1	B	11	ASP	2.3
1	F	13	PRO	2.3
1	F	80	PRO	2.3
1	C	100	SER	2.3
1	D	81	ASN	2.3
1	D	10	LEU	2.3
2	H	477	TYR	2.2
1	C	10	LEU	2.2
1	A	124	GLU	2.2
1	A	35	PRO	2.2
1	F	40	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	106	TRP	2.2
2	L	473	GLU	2.2
2	K	477	TYR	2.2
1	E	67	VAL	2.2
1	A	8	LEU	2.2
2	L	481	SER	2.2
1	C	23	THR	2.2
1	E	78	TYR	2.2
2	L	476	PHE	2.2
1	E	121	CYS	2.2
1	F	67	VAL	2.2
1	B	27	THR	2.1
1	E	84	SER	2.1
1	D	96	PRO	2.1
1	E	111	PRO	2.1
1	E	94	PHE	2.1
1	F	108	GLU	2.1
1	A	109	ALA	2.1
1	B	76	PHE	2.1
1	B	113	GLU	2.1
1	D	105	VAL	2.1
1	A	53[A]	CYS	2.1
1	D	61	ILE	2.1
1	D	93	ILE	2.1
1	E	8	LEU	2.1
1	E	62	ASP	2.1
1	F	33	GLN	2.1
1	B	78	TYR	2.1
1	C	40	VAL	2.1
1	B	37	ASP	2.1
1	C	121	CYS	2.1
1	D	16	LEU	2.1
1	F	16	LEU	2.1
1	A	108	GLU	2.0
1	C	113	GLU	2.0
1	F	78	TYR	2.0
1	A	76	PHE	2.0
1	F	8	LEU	2.0
1	F	109	ALA	2.0
1	F	27	THR	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 monosaccharides 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.