



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:58 PM UTC

PDB ID : 3WJ2 / pdb_00003wj2
Title : Crystal structure of ESTFA (FE-lacking apo form)
Authors : Ohara, K.; Unno, H.; Oshima, Y.; Furukawa, K.; Fujino, N.; Hirooka, K.; Hemmi, H.; Takahashi, S.; Nishino, T.; Kusunoki, M.; Nakayama, T.
Deposited on : 2013-10-03
Resolution : 1.61 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

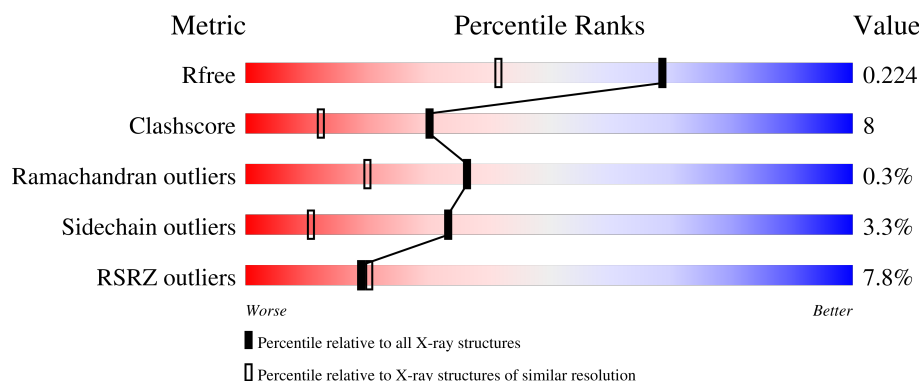
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	308	2% 76% 18% ...
1	B	308	3% 73% 21% ...
1	C	308	9% 81% 14% ...
1	D	308	15% 73% 22% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10427 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 Carboxylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2355	1502	394	446	13			
1	B	300	Total	C	N	O	S	0	0	0
			2363	1506	396	448	13			
1	C	300	Total	C	N	O	S	0	0	0
			2363	1506	396	448	13			
1	D	300	Total	C	N	O	S	0	0	0
			2363	1506	396	448	13			

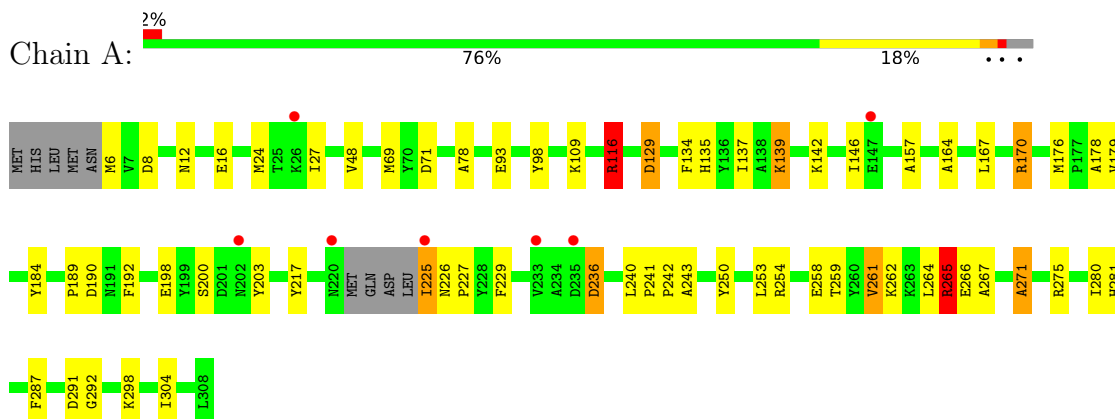
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	286	Total	O	0	0
			286	286		
2	B	284	Total	O	0	0
			284	284		
2	C	219	Total	O	0	0
			219	219		
2	D	194	Total	O	0	0
			194	194		

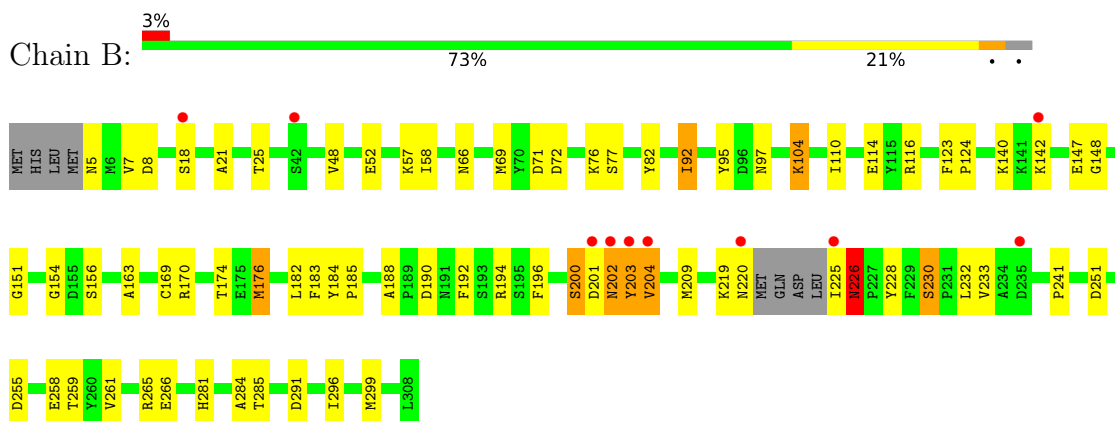
3 Residue-property plots [i](#)

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.

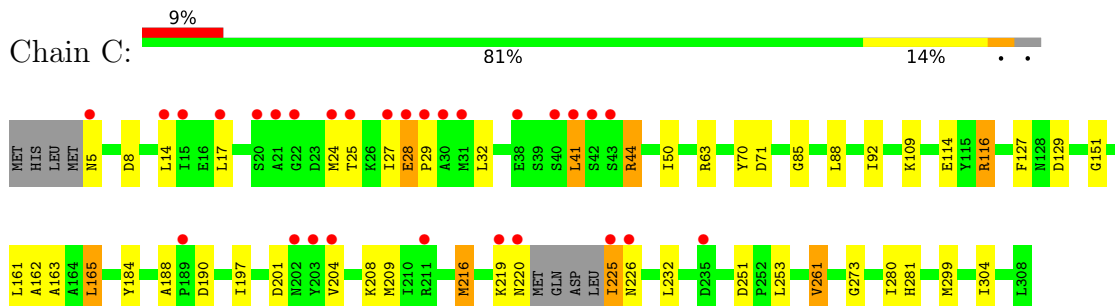
• Molecule 1: Carboxylesterase



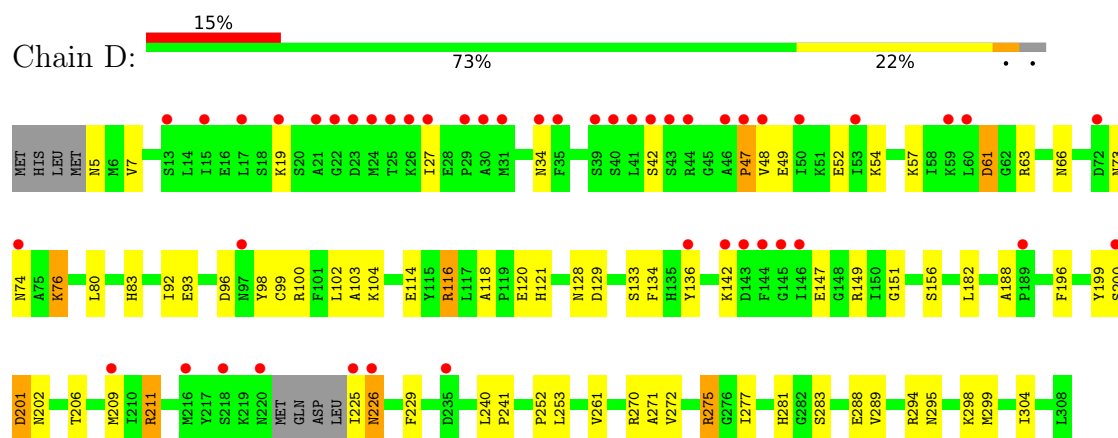
• Molecule 1: Carboxylesterase



• Molecule 1: Carboxylesterase



● Molecule 1: Carboxylesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.80Å 137.36Å 76.88Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	46.37 – 1.61 46.37 – 1.61	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.37-1.61) 99.0 (46.37-1.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.188 , 0.225 0.186 , 0.224	Depositor DCC
R_{free} test set	8382 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10427	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	1.68	28/2406 (1.2%)	1.59	29/3245 (0.9%)
1	B	1.75	30/2414 (1.2%)	1.54	21/3256 (0.6%)
1	C	1.58	13/2414 (0.5%)	1.44	15/3256 (0.5%)
1	D	1.59	21/2414 (0.9%)	1.50	22/3256 (0.7%)
All	All	1.65	92/9648 (1.0%)	1.52	87/13013 (0.7%)

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	261	VAL	CA-CB	10.58	1.66	1.54
1	B	151	GLY	N-CA	8.92	1.52	1.44
1	B	226	ASN	N-CA	-8.82	1.35	1.46
1	B	176	MET	CB-CG	8.28	1.77	1.52
1	C	184	TYR	CA-CB	7.96	1.59	1.52
1	B	190	ASP	N-CA	7.95	1.55	1.46
1	B	261	VAL	CA-CB	7.89	1.63	1.54
1	B	183	PHE	CA-CB	7.36	1.62	1.53
1	A	241	PRO	CA-C	7.34	1.57	1.52
1	C	151	GLY	N-CA	7.27	1.51	1.44
1	B	58	ILE	CA-CB	7.20	1.62	1.53
1	B	170	ARG	C-O	7.19	1.32	1.24
1	D	271	ALA	N-CA	6.94	1.54	1.46
1	A	78	ALA	N-CA	6.78	1.54	1.45
1	D	188	ALA	CA-CB	6.67	1.62	1.53
1	D	156	SER	CA-C	6.61	1.59	1.52
1	C	70	TYR	N-CA	6.57	1.54	1.46
1	A	184	TYR	C-O	6.51	1.27	1.23
1	A	262	LYS	N-CA	6.50	1.54	1.46
1	B	184	TYR	C-O	6.42	1.27	1.23
1	B	154	GLY	N-CA	6.30	1.52	1.45
1	B	204	VAL	C-O	-6.30	1.18	1.24
1	D	7	VAL	CA-CB	6.27	1.60	1.54
1	A	292	GLY	C-O	6.27	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	TYR	N-CA	6.19	1.53	1.46
1	A	164	ALA	N-CA	6.12	1.53	1.46
1	D	133	SER	C-O	-6.11	1.17	1.24
1	A	179	VAL	N-CA	6.10	1.52	1.46
1	A	48	VAL	CA-CB	5.94	1.61	1.54
1	D	241	PRO	CA-C	5.94	1.56	1.52
1	D	103	ALA	N-CA	-5.92	1.39	1.46
1	A	267	ALA	CA-CB	5.90	1.63	1.53
1	A	250	TYR	N-CA	5.90	1.55	1.46
1	B	255	ASP	N-CA	5.90	1.52	1.46
1	B	95	TYR	CA-CB	5.88	1.64	1.53
1	D	252	PRO	N-CA	-5.85	1.39	1.47
1	D	96	ASP	N-CA	-5.83	1.39	1.46
1	A	265	ARG	CD-NE	-5.82	1.38	1.46
1	D	134	PHE	CA-CB	5.81	1.62	1.53
1	C	50	ILE	CA-CB	5.79	1.62	1.54
1	B	296	ILE	N-CA	5.78	1.53	1.46
1	B	7	VAL	N-CA	5.75	1.52	1.46
1	B	77	SER	N-CA	5.71	1.53	1.45
1	A	129	ASP	N-CA	-5.66	1.39	1.46
1	A	298	LYS	N-CA	5.64	1.53	1.46
1	D	188	ALA	N-CA	5.63	1.50	1.45
1	A	304	ILE	CA-C	5.54	1.59	1.52
1	D	199	TYR	CA-C	5.52	1.60	1.52
1	C	226	ASN	N-CA	5.46	1.53	1.45
1	A	271	ALA	CA-CB	-5.42	1.44	1.53
1	D	96	ASP	CA-CB	5.39	1.61	1.53
1	B	21	ALA	CA-CB	5.37	1.62	1.53
1	B	182	LEU	CA-CB	5.35	1.61	1.53
1	B	8	ASP	CA-C	5.34	1.59	1.53
1	B	97	ASN	CA-C	5.34	1.59	1.52
1	C	162	ALA	CA-CB	5.32	1.61	1.53
1	A	287	PHE	CA-C	5.30	1.60	1.52
1	A	229	PHE	CA-CB	5.29	1.62	1.53
1	C	190	ASP	N-CA	5.28	1.52	1.46
1	A	280	ILE	C-O	5.28	1.29	1.23
1	A	203	TYR	CA-CB	5.25	1.60	1.53
1	C	85	GLY	N-CA	5.25	1.52	1.45
1	B	82	TYR	CA-CB	5.25	1.60	1.53
1	B	266	GLU	C-O	5.25	1.30	1.24
1	B	184	TYR	CA-CB	5.24	1.57	1.52
1	B	110	ILE	CA-CB	5.24	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	261	VAL	CB-CG1	-5.23	1.35	1.52
1	A	8	ASP	CA-C	5.22	1.59	1.53
1	A	135	HIS	N-CA	5.22	1.52	1.46
1	B	174	THR	N-CA	-5.21	1.39	1.45
1	D	136	TYR	N-CA	5.20	1.52	1.46
1	D	299	MET	CG-SD	5.20	1.93	1.80
1	A	98	TYR	CA-C	5.19	1.59	1.52
1	B	259	THR	N-CA	5.18	1.52	1.46
1	B	266	GLU	N-CA	5.15	1.52	1.46
1	A	178	ALA	N-CA	5.14	1.52	1.46
1	A	266	GLU	N-CA	5.14	1.52	1.46
1	C	273	GLY	N-CA	5.13	1.50	1.45
1	C	8	ASP	CA-C	5.12	1.59	1.53
1	D	151	GLY	N-CA	5.11	1.49	1.44
1	A	265	ARG	CZ-NH1	-5.10	1.25	1.32
1	A	243	ALA	CA-CB	-5.10	1.42	1.53
1	B	176	MET	CA-CB	5.10	1.61	1.53
1	C	280	ILE	CG1-CD1	5.09	1.71	1.51
1	B	291	ASP	N-CA	-5.08	1.40	1.46
1	D	182	LEU	N-CA	-5.07	1.40	1.46
1	D	99	CYS	C-O	-5.06	1.18	1.24
1	D	118	ALA	CA-CB	5.04	1.60	1.53
1	C	304	ILE	N-CA	5.03	1.52	1.46
1	A	137	ILE	CA-CB	5.03	1.61	1.54
1	B	92	ILE	N-CA	-5.01	1.40	1.46
1	A	157	ALA	N-CA	5.00	1.52	1.46

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH1	-13.97	107.53	121.50
1	A	304	ILE	O-C-N	10.32	127.03	120.42
1	B	299	MET	CG-SD-CE	-10.02	78.86	100.90
1	A	116	ARG	NE-CZ-NH2	-9.97	110.23	119.20
1	A	116	ARG	CD-NE-CZ	9.49	137.69	124.40
1	C	201	ASP	N-CA-C	9.16	124.44	112.72
1	C	219	LYS	CA-C-N	8.79	137.52	121.70
1	C	219	LYS	C-N-CA	8.79	137.52	121.70
1	A	116	ARG	NE-CZ-NH1	8.78	130.28	121.50
1	A	265	ARG	NE-CZ-NH2	8.76	127.08	119.20
1	D	240	LEU	CA-C-N	-8.46	113.57	119.66
1	D	240	LEU	C-N-CA	-8.46	113.57	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	241	PRO	O-C-N	8.20	125.00	121.15
1	A	265	ARG	CD-NE-CZ	-8.07	113.09	124.40
1	B	200	SER	CA-C-N	-8.07	109.63	121.98
1	B	200	SER	C-N-CA	-8.07	109.63	121.98
1	B	176	MET	CB-CG-SD	-8.01	88.68	112.70
1	D	283	SER	N-CA-C	7.62	120.25	111.11
1	C	219	LYS	N-CA-C	7.46	119.11	110.97
1	D	288	GLU	CA-C-N	7.34	130.14	121.84
1	D	288	GLU	C-N-CA	7.34	130.14	121.84
1	B	204	VAL	N-CA-CB	6.91	118.93	110.64
1	A	265	ARG	CB-CG-CD	6.85	127.05	111.30
1	D	226	ASN	CB-CA-C	6.74	118.57	108.86
1	A	93	GLU	N-CA-C	6.62	118.49	111.28
1	A	258	GLU	N-CA-C	-6.57	104.20	111.36
1	A	254	ARG	CA-C-N	-6.55	111.91	120.09
1	A	254	ARG	C-N-CA	-6.55	111.91	120.09
1	B	116	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	B	203	TYR	N-CA-C	6.30	124.23	110.80
1	C	220	ASN	N-CA-C	6.26	128.53	111.00
1	A	264	LEU	N-CA-C	-6.19	104.45	111.07
1	A	241	PRO	O-C-N	6.15	124.04	121.15
1	B	163	ALA	N-CA-C	-6.14	104.66	111.36
1	D	275	ARG	NE-CZ-NH1	-6.13	115.37	121.50
1	A	190	ASP	N-CA-C	6.03	118.66	107.99
1	D	304	ILE	CA-C-N	-5.98	113.46	119.56
1	D	304	ILE	C-N-CA	-5.98	113.46	119.56
1	C	216	MET	CG-SD-CE	-5.95	87.81	100.90
1	C	219	LYS	CA-C-O	-5.93	114.77	121.00
1	A	116	ARG	CG-CD-NE	-5.92	98.98	112.00
1	C	190	ASP	N-CA-C	5.90	118.35	108.02
1	A	292	GLY	N-CA-C	-5.83	105.31	112.77
1	C	163	ALA	O-C-N	5.82	128.79	122.15
1	A	259	THR	O-C-N	-5.74	116.16	122.07
1	B	226	ASN	O-C-N	5.73	125.87	121.23
1	A	98	TYR	CA-C-O	-5.71	114.82	120.70
1	D	83	HIS	N-CA-C	5.70	118.11	110.35
1	C	226	ASN	O-C-N	5.68	126.31	121.20
1	A	176	MET	CA-C-N	-5.67	113.85	119.92
1	A	176	MET	C-N-CA	-5.67	113.85	119.92
1	B	176	MET	CG-SD-CE	-5.66	88.45	100.90
1	C	184	TYR	O-C-N	5.65	124.13	121.53
1	B	265	ARG	O-C-N	5.65	128.59	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	GLU	N-CA-C	-5.65	105.27	111.82
1	A	134	PHE	O-C-N	5.63	127.87	122.07
1	B	265	ARG	CA-C-O	-5.56	114.52	120.42
1	D	102	LEU	N-CA-C	5.55	117.01	111.07
1	B	285	THR	N-CA-C	-5.52	106.50	113.18
1	C	116	ARG	CA-CB-CG	-5.51	103.08	114.10
1	D	261	VAL	CB-CA-C	-5.45	104.90	111.88
1	C	251	ASP	CA-C-O	5.44	124.77	119.22
1	C	261	VAL	CB-CA-C	5.43	121.06	112.26
1	A	184	TYR	O-C-N	-5.43	119.03	121.53
1	B	261	VAL	CB-CA-C	-5.40	104.97	111.88
1	A	146	ILE	N-CA-C	5.37	116.10	107.73
1	B	185	PRO	CB-CA-C	-5.37	103.92	110.95
1	D	229	PHE	N-CA-C	-5.37	104.99	112.45
1	D	206	THR	CA-C-N	5.36	126.03	120.03
1	D	206	THR	C-N-CA	5.36	126.03	120.03
1	B	284	ALA	O-C-N	5.34	127.79	122.12
1	D	272	VAL	CA-C-N	-5.34	118.02	121.65
1	D	272	VAL	C-N-CA	-5.34	118.02	121.65
1	B	194	ARG	CA-C-N	-5.32	112.74	120.29
1	B	194	ARG	C-N-CA	-5.32	112.74	120.29
1	D	116	ARG	NE-CZ-NH1	-5.32	116.19	121.50
1	B	230	SER	CA-C-N	5.22	125.03	119.28
1	B	230	SER	C-N-CA	5.22	125.03	119.28
1	A	261	VAL	O-C-N	5.11	126.82	121.87
1	A	164	ALA	N-CA-C	-5.06	105.85	111.36
1	A	229	PHE	N-CA-C	-5.06	104.76	112.04
1	C	299	MET	CB-CG-SD	-5.06	97.53	112.70
1	D	295	ASN	CA-C-O	-5.06	115.06	120.42
1	D	199	TYR	N-CA-C	-5.05	105.85	112.41
1	D	47	PRO	N-CA-C	-5.01	103.32	111.19
1	A	241	PRO	CA-C-N	5.01	126.10	119.84
1	A	241	PRO	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2355	0	2318	39	0
1	B	2363	0	2324	53	0
1	C	2363	0	2324	27	0
1	D	2363	0	2324	45	0
2	A	286	0	0	15	0
2	B	284	0	0	15	0
2	C	219	0	0	2	0
2	D	194	0	0	16	0
All	All	10427	0	9290	158	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 (158) 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:B:176:MET:CB	1:B:176:MET:CG	1.77	1.59
1:B:69:MET:HG3	2:B:449:HOH:O	1.09	1.24
1:A:116:ARG:HD3	1:A:129:ASP:OD2	1.41	1.21
1:A:116:ARG:CD	1:A:129:ASP:OD2	1.92	1.17
1:B:219:LYS:HE2	2:B:512:HOH:O	1.52	1.09
1:A:225:ILE:HD13	1:A:225:ILE:O	1.54	1.08
1:C:116:ARG:NH1	1:C:129:ASP:OD1	1.87	1.07
1:D:48:VAL:CG1	1:D:104:LYS:HD2	1.88	1.01
1:D:63:ARG:HG3	1:D:116:ARG:NH1	1.77	0.99
1:B:176:MET:CB	1:B:176:MET:SD	2.50	0.98
1:A:170:ARG:NH2	1:A:236:ASP:O	1.97	0.96
1:B:69:MET:CG	2:B:449:HOH:O	1.80	0.96
1:B:220:ASN:C	2:B:451:HOH:O	2.11	0.93
1:B:201:ASP:O	1:B:203:TYR:N	2.01	0.93
1:B:5:ASN:N	2:B:661:HOH:O	1.99	0.93
1:D:128:ASN:ND2	2:D:577:HOH:O	2.02	0.91
1:A:116:ARG:HD2	1:A:129:ASP:OD2	1.72	0.89
1:D:48:VAL:HG11	1:D:104:LYS:HD2	1.56	0.88
1:A:225:ILE:O	1:A:225:ILE:CD1	2.21	0.87
1:D:5:ASN:N	2:D:448:HOH:O	2.07	0.87
1:D:48:VAL:HG13	1:D:104:LYS:HD2	1.55	0.85
1:D:34:ASN:HB2	2:D:456:HOH:O	1.76	0.85
1:A:291:ASP:OD2	1:D:270:ARG:HD2	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:OD2	1:B:104:LYS:HE3	1.76	0.83
1:B:204:VAL:HB	2:B:634:HOH:O	1.77	0.83
1:A:265:ARG:HD2	1:A:271:ALA:HB3	1.61	0.83
1:D:120:GLU:HG3	2:D:455:HOH:O	1.79	0.82
1:C:116:ARG:NH1	1:C:129:ASP:CG	2.38	0.81
1:B:176:MET:HE1	1:B:241:PRO:HD3	1.64	0.79
1:C:14:LEU:HD22	1:C:204:VAL:HG21	1.64	0.79
1:B:201:ASP:C	1:B:203:TYR:H	1.92	0.77
1:B:176:MET:SD	1:B:176:MET:HB3	2.26	0.75
1:C:24:MET:HE2	1:C:209:MET:HE2	1.67	0.75
1:D:34:ASN:HB2	2:D:570:HOH:O	1.86	0.74
1:A:265:ARG:NH1	2:A:448:HOH:O	2.01	0.74
1:C:63:ARG:HG3	1:C:116:ARG:NH1	2.03	0.73
1:D:116:ARG:HD2	1:D:121:HIS:CE1	2.24	0.72
1:C:32:LEU:HD21	1:C:209:MET:HE1	1.72	0.72
1:A:265:ARG:NH2	2:A:448:HOH:O	2.24	0.71
1:A:225:ILE:O	1:A:225:ILE:CG1	2.39	0.70
1:D:63:ARG:HG3	1:D:116:ARG:HH12	1.51	0.70
1:B:176:MET:HB3	1:B:176:MET:HE2	1.73	0.70
1:A:227:PRO:HD3	2:A:578:HOH:O	1.91	0.69
1:B:5:ASN:N	2:B:561:HOH:O	2.25	0.69
1:B:76:LYS:HG3	1:B:147:GLU:HB2	1.75	0.69
1:A:265:ARG:CZ	2:A:448:HOH:O	2.38	0.68
1:B:57:LYS:NZ	1:B:66:ASN:HD21	1.90	0.68
1:C:14:LEU:CD2	1:C:204:VAL:HG21	2.24	0.68
1:B:226:ASN:HD22	1:B:228:TYR:H	1.42	0.67
1:A:24:MET:HB3	1:A:27:ILE:HD12	1.75	0.67
1:A:225:ILE:HA	2:A:515:HOH:O	1.94	0.67
1:C:71:ASP:OD1	1:C:109:LYS:NZ	2.27	0.66
1:A:198:GLU:O	1:C:5:ASN:N	2.29	0.65
1:B:176:MET:CB	1:B:176:MET:HE2	2.26	0.65
2:A:565:HOH:O	1:B:233:VAL:HG12	1.96	0.64
1:D:209:MET:HG3	2:D:445:HOH:O	1.97	0.64
1:C:63:ARG:HE	1:C:116:ARG:HH12	1.46	0.64
1:C:225:ILE:HG22	1:C:225:ILE:O	1.99	0.63
1:B:176:MET:HB3	1:B:176:MET:CE	2.29	0.62
1:B:176:MET:CB	1:B:176:MET:CE	2.77	0.62
1:B:176:MET:HE1	1:B:241:PRO:CD	2.31	0.61
1:C:116:ARG:NH1	1:C:129:ASP:OD2	2.33	0.61
1:B:196:PHE:O	1:B:200:SER:HB3	2.01	0.61
1:B:52:GLU:HG3	1:B:71:ASP:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ILE:N	2:D:419:HOH:O	2.33	0.60
1:A:71:ASP:OD2	1:A:109:LYS:NZ	2.34	0.60
1:A:226:ASN:HA	2:A:578:HOH:O	2.01	0.60
1:D:19:LYS:HD3	1:D:202:ASN:HD22	1.64	0.60
1:D:225:ILE:HA	2:D:419:HOH:O	2.01	0.59
1:D:270:ARG:HD3	2:D:545:HOH:O	2.01	0.59
1:B:201:ASP:C	1:B:201:ASP:OD1	2.46	0.58
1:B:48:VAL:CG1	1:B:104:LYS:HD2	2.34	0.58
1:B:200:SER:OG	2:B:545:HOH:O	2.14	0.57
1:D:63:ARG:HE	1:D:116:ARG:HH12	1.51	0.57
1:A:167:LEU:HD23	1:A:240:LEU:HD21	1.86	0.57
1:A:253:LEU:HD12	1:A:281:HIS:CE1	2.39	0.57
1:C:253:LEU:HD12	1:C:281:HIS:CE1	2.40	0.57
1:D:57:LYS:NZ	1:D:66:ASN:HD21	2.02	0.57
1:B:220:ASN:ND2	2:B:655:HOH:O	2.25	0.57
1:D:49:GLU:O	1:D:104:LYS:HE2	2.05	0.56
1:A:217:TYR:OH	2:A:652:HOH:O	2.09	0.56
1:B:140:LYS:HD3	2:B:572:HOH:O	2.05	0.56
1:D:142:LYS:NZ	2:D:573:HOH:O	2.15	0.56
1:A:116:ARG:CD	1:A:129:ASP:CG	2.75	0.56
1:B:76:LYS:HG2	1:B:148:GLY:N	2.21	0.55
1:D:48:VAL:HG13	1:D:104:LYS:CD	2.33	0.55
1:D:48:VAL:CG1	1:D:104:LYS:CD	2.75	0.55
1:A:170:ARG:HG2	2:A:609:HOH:O	2.06	0.55
1:A:116:ARG:HD2	1:A:129:ASP:CG	2.29	0.55
1:B:230:SER:O	1:B:233:VAL:HG22	2.07	0.54
1:D:76:LYS:HE2	2:D:550:HOH:O	2.08	0.54
1:D:120:GLU:CG	2:D:455:HOH:O	2.46	0.53
1:C:188:ALA:HB2	1:C:232:LEU:HD12	1.90	0.53
1:B:57:LYS:HZ3	1:B:66:ASN:HD21	1.56	0.52
1:B:76:LYS:HA	2:B:640:HOH:O	2.09	0.52
1:C:24:MET:CE	1:C:209:MET:HE2	2.39	0.52
1:A:142:LYS:HG2	2:A:659:HOH:O	2.09	0.52
1:B:25:THR:HG22	1:B:209:MET:SD	2.50	0.51
1:B:202:ASN:O	2:B:663:HOH:O	2.19	0.51
1:D:92:ILE:HG13	1:D:114:GLU:HG3	1.92	0.51
1:B:188:ALA:HB2	1:B:232:LEU:HD12	1.92	0.51
1:D:63:ARG:HG3	1:D:116:ARG:HH11	1.72	0.50
1:C:5:ASN:OD1	1:C:5:ASN:C	2.53	0.50
1:C:225:ILE:HD12	1:C:225:ILE:N	2.26	0.50
1:D:57:LYS:HZ3	1:D:66:ASN:HD21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:PHE:O	1:D:200:SER:HB3	2.12	0.50
1:B:57:LYS:HZ2	1:B:66:ASN:HD21	1.61	0.49
1:B:251:ASP:OD2	1:B:281:HIS:HD2	1.97	0.48
1:C:28:GLU:HG3	1:C:29:PRO:N	2.27	0.48
1:D:93:GLU:HG2	2:D:513:HOH:O	2.12	0.48
1:B:176:MET:HE1	1:B:241:PRO:CG	2.43	0.48
1:C:253:LEU:HD12	1:C:281:HIS:HE1	1.79	0.48
1:C:209:MET:HG3	2:C:510:HOH:O	2.14	0.47
1:D:76:LYS:HG2	1:D:147:GLU:HB2	1.94	0.47
1:A:227:PRO:CD	2:A:578:HOH:O	2.55	0.47
1:B:156:SER:OG	1:B:281:HIS:HE1	1.97	0.47
1:A:6:MET:N	2:A:664:HOH:O	2.48	0.47
1:A:189:PRO:HG3	2:A:515:HOH:O	2.14	0.46
1:D:5:ASN:CA	2:D:448:HOH:O	2.59	0.46
1:A:139:LYS:HB2	1:A:139:LYS:HE2	1.49	0.46
1:B:201:ASP:C	1:B:203:TYR:N	2.59	0.45
1:C:225:ILE:HA	2:C:596:HOH:O	2.16	0.45
1:D:211:ARG:HD2	1:D:211:ARG:HA	1.69	0.45
1:B:123:PHE:CD1	1:B:124:PRO:HA	2.52	0.45
1:B:5:ASN:C	2:B:661:HOH:O	2.59	0.45
1:B:226:ASN:ND2	1:B:228:TYR:H	2.13	0.45
1:D:201:ASP:HB2	2:D:481:HOH:O	2.17	0.45
1:A:12:ASN:O	1:A:16:GLU:HG2	2.17	0.45
1:B:18:SER:OG	1:B:203:TYR:O	2.35	0.45
1:A:275:ARG:HB3	1:D:275:ARG:HB3	1.99	0.44
1:C:25:THR:HG21	1:C:208:LYS:HG2	1.99	0.44
1:D:116:ARG:NH1	1:D:129:ASP:OD1	2.50	0.44
1:B:69:MET:SD	1:B:71:ASP:HB2	2.58	0.44
1:D:47:PRO:HB3	1:D:100:ARG:CD	2.47	0.44
1:D:73:ASN:O	1:D:74:ASN:C	2.60	0.44
1:A:225:ILE:HD13	1:A:225:ILE:C	2.36	0.43
1:A:69:MET:HE3	2:A:480:HOH:O	2.18	0.43
1:A:170:ARG:NH2	1:A:236:ASP:C	2.74	0.42
1:A:192:PHE:CZ	1:B:192:PHE:CZ	3.06	0.42
1:C:127:PHE:HA	1:C:161:LEU:HD22	2.01	0.42
1:D:63:ARG:NE	1:D:116:ARG:HH12	2.17	0.42
1:D:63:ARG:CG	1:D:116:ARG:NH1	2.66	0.42
1:A:265:ARG:HH11	1:A:265:ARG:HD3	1.19	0.42
1:B:92:ILE:HG13	1:B:114:GLU:HG3	2.01	0.42
1:B:202:ASN:C	2:B:663:HOH:O	2.62	0.41
1:B:209:MET:HG3	2:B:406:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ARG:HD2	1:D:121:HIS:ND1	2.34	0.41
1:C:41:LEU:O	1:C:44:ARG:HB2	2.20	0.41
1:A:225:ILE:N	2:A:658:HOH:O	2.54	0.41
1:B:196:PHE:O	1:B:200:SER:CB	2.69	0.41
1:C:92:ILE:HG13	1:C:114:GLU:HG3	2.03	0.41
1:C:165:LEU:C	1:C:165:LEU:HD12	2.46	0.41
1:B:169:CYS:HB3	1:B:176:MET:HG2	2.03	0.41
1:D:253:LEU:HD12	1:D:281:HIS:CE1	2.55	0.41
1:A:6:MET:HG3	1:C:197:ILE:HG13	2.03	0.40
1:A:261:VAL:HG21	1:D:277:ILE:HG21	2.03	0.40
1:D:294:ARG:O	1:D:298:LYS:HG3	2.21	0.40
1:D:209:MET:CG	2:D:445:HOH:O	2.65	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	295/308 (96%)	286 (97%)	9 (3%)	0	100	100
1	B	296/308 (96%)	287 (97%)	8 (3%)	1 (0%)	36	20
1	C	296/308 (96%)	283 (96%)	13 (4%)	0	100	100
1	D	296/308 (96%)	275 (93%)	19 (6%)	2 (1%)	18	6
All	All	1183/1232 (96%)	1131 (96%)	49 (4%)	3 (0%)	36	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	ASN
1	D	42	SER
1	D	61	ASP

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	251/260 (96%)	243 (97%)	8 (3%)	34	11
1	B	252/260 (97%)	248 (98%)	4 (2%)	55	32
1	C	252/260 (97%)	242 (96%)	10 (4%)	28	7
1	D	252/260 (97%)	241 (96%)	11 (4%)	25	6
All	All	1007/1040 (97%)	974 (97%)	33 (3%)	33	11

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	139	LYS
1	A	170	ARG
1	A	200	SER
1	A	225	ILE
1	A	236	ASP
1	A	242	PRO
1	A	265	ARG
1	B	104	LYS
1	B	142	LYS
1	B	225	ILE
1	B	226	ASN
1	C	17	LEU
1	C	27	ILE
1	C	28	GLU
1	C	41	LEU
1	C	44	ARG
1	C	88	LEU
1	C	165	LEU
1	C	216	MET
1	C	225	ILE
1	C	261	VAL
1	D	27	ILE
1	D	52	GLU

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Mol	Chain	Res	Type
1	D	54	LYS
1	D	61	ASP
1	D	76	LYS
1	D	80	LEU
1	D	149	ARG
1	D	201	ASP
1	D	211	ARG
1	D	226	ASN
1	D	289	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	121	HIS
1	A	180	GLN
1	A	248	ASN
1	A	295	ASN
1	B	66	ASN
1	B	121	HIS
1	B	226	ASN
1	B	281	HIS
1	B	295	ASN
1	C	34	ASN
1	C	226	ASN
1	C	295	ASN
1	D	34	ASN
1	D	66	ASN
1	D	128	ASN
1	D	160	ASN
1	D	180	GLN
1	D	202	ASN
1	D	248	ASN
1	D	295	ASN

5.3.3 RNA ⓘ

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	299/308 (97%)	0.11	7 (2%) 61 65	9, 20, 35, 48	0
1	B	300/308 (97%)	-0.06	10 (3%) 49 53	8, 17, 34, 43	0
1	C	300/308 (97%)	0.34	29 (9%) 13 14	10, 21, 46, 67	0
1	D	300/308 (97%)	0.84	47 (15%) 5 4	11, 25, 52, 78	0
All	All	1199/1232 (97%)	0.31	93 (7%) 19 20	8, 21, 42, 78	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	ILE	7.2
1	D	27	ILE	6.4
1	C	225	ILE	6.0
1	B	203	TYR	5.1
1	D	31	MET	5.0
1	D	34	ASN	4.9
1	A	225	ILE	4.8
1	D	46	ALA	4.7
1	D	225	ILE	4.4
1	D	220	ASN	4.3
1	A	220	ASN	4.1
1	B	202	ASN	4.0
1	D	17	LEU	3.9
1	D	42	SER	3.9
1	D	47	PRO	3.7
1	D	43	SER	3.6
1	D	35	PHE	3.5
1	B	220	ASN	3.4
1	C	20	SER	3.4
1	D	25	THR	3.2
1	D	50	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	202	ASN	3.2
1	A	235	ASP	3.2
1	C	189	PRO	3.2
1	D	21	ALA	3.2
1	C	5	ASN	3.1
1	C	17	LEU	3.1
1	D	19	LYS	3.0
1	D	146	ILE	3.0
1	C	43	SER	3.0
1	C	25	THR	3.0
1	D	53	ILE	3.0
1	D	144	PHE	3.0
1	C	204	VAL	2.9
1	D	40	SER	2.9
1	D	24	MET	2.9
1	C	220	ASN	2.9
1	D	145	GLY	2.9
1	C	235	ASP	2.9
1	D	29	PRO	2.9
1	D	218	SER	2.8
1	C	24	MET	2.8
1	C	226	ASN	2.7
1	B	201	ASP	2.7
1	D	60	LEU	2.6
1	A	233	VAL	2.6
1	C	42	SER	2.6
1	C	31	MET	2.6
1	D	74	ASN	2.6
1	D	209	MET	2.6
1	D	235	ASP	2.5
1	B	42	SER	2.5
1	D	44	ARG	2.5
1	D	200	SER	2.5
1	D	22	GLY	2.5
1	D	136	TYR	2.4
1	C	27	ILE	2.4
1	D	23	ASP	2.4
1	C	38	GLU	2.4
1	C	41	LEU	2.4
1	D	226	ASN	2.3
1	C	219	LYS	2.3
1	B	142	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	216	MET	2.3
1	D	41	LEU	2.3
1	D	26	LYS	2.3
1	D	72	ASP	2.3
1	D	189	PRO	2.3
1	C	22	GLY	2.3
1	C	30	ALA	2.2
1	A	202	ASN	2.2
1	C	14	LEU	2.2
1	D	142	LYS	2.2
1	C	203	TYR	2.2
1	D	48	VAL	2.2
1	D	30	ALA	2.2
1	A	26	LYS	2.2
1	B	235	ASP	2.1
1	B	204	VAL	2.1
1	C	28	GLU	2.1
1	A	147	GLU	2.1
1	C	29	PRO	2.1
1	D	15	ILE	2.1
1	D	59	LYS	2.1
1	D	13	SER	2.1
1	C	21	ALA	2.1
1	D	143	ASP	2.1
1	C	211	ARG	2.1
1	B	18	SER	2.0
1	D	97	ASN	2.0
1	C	15	ILE	2.0
1	C	40	SER	2.0
1	D	39	SER	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 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.