



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:09 PM GMT

PDB ID : 1E8F
Title : STRUCTURE OF THE H61T MUTANT OF THE FLAVOENZYME
VANILLYL-ALCOHOL OXIDASE IN THE APO FORM
Authors : Mattevi, A.; Fraaije, M.W.
Deposited on : 2000-09-20
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

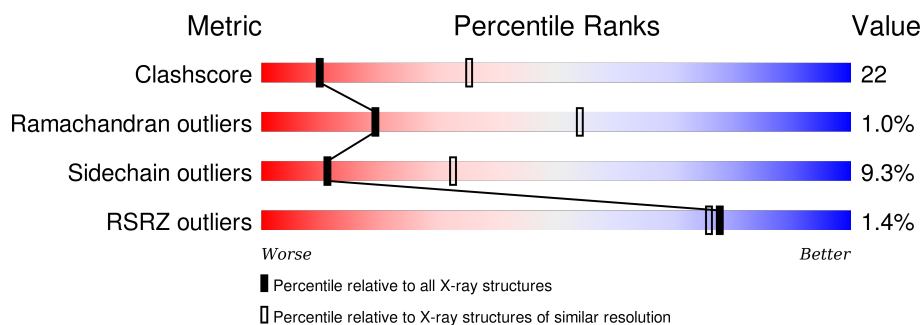
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	<div> <div> <div></div> <div>46%</div> <div>41%</div> <div>8%</div> <div>...</div> </div> </div>
1	B	560	<div> <div> <div></div> <div>49%</div> <div>40%</div> <div>8%</div> <div>...</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8642 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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	136	0	0
			4311	2768	737	782	24			
1	B	545	Total	C	N	O	S	136	0	0
			4311	2768	737	782	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	THR	HIS	ENGINEERED	UNP P56216
B	61	THR	HIS	ENGINEERED	UNP P56216

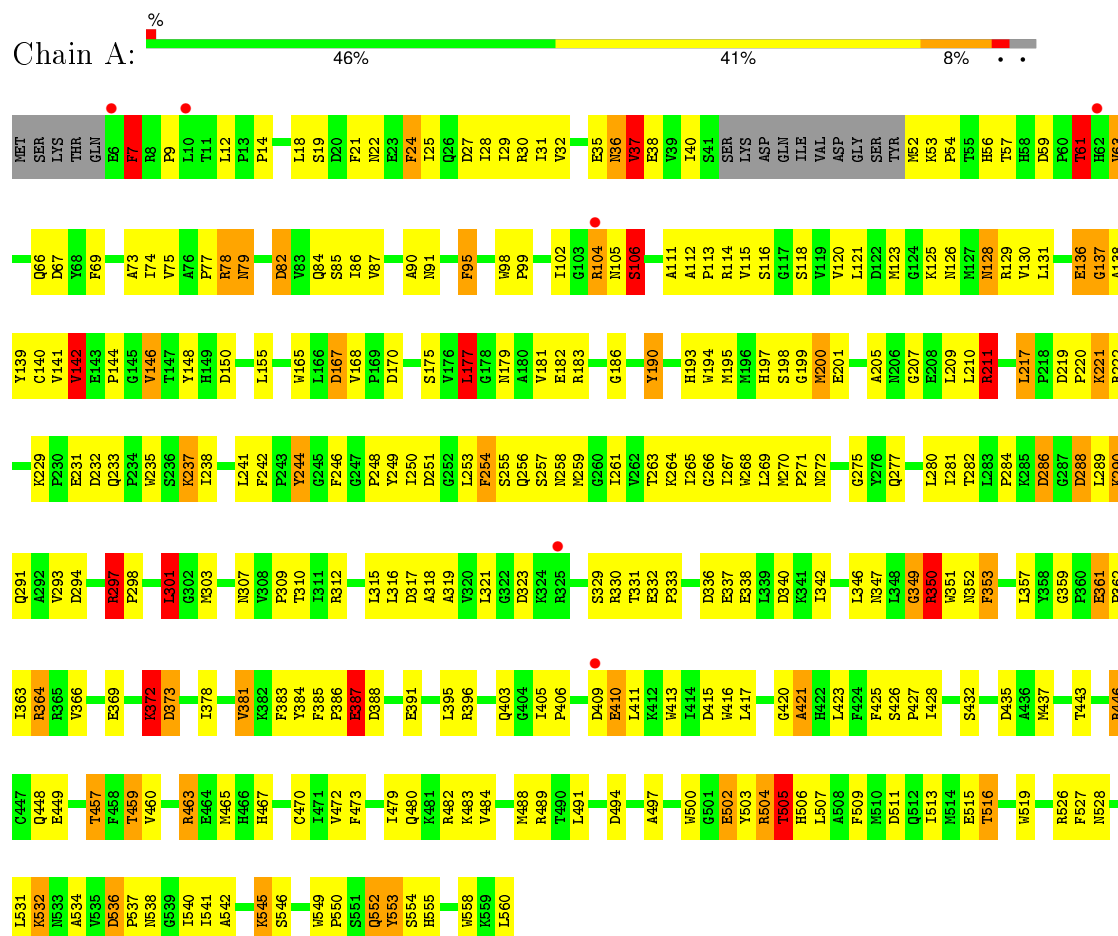
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	8	Total	O	0	0
			8	8		

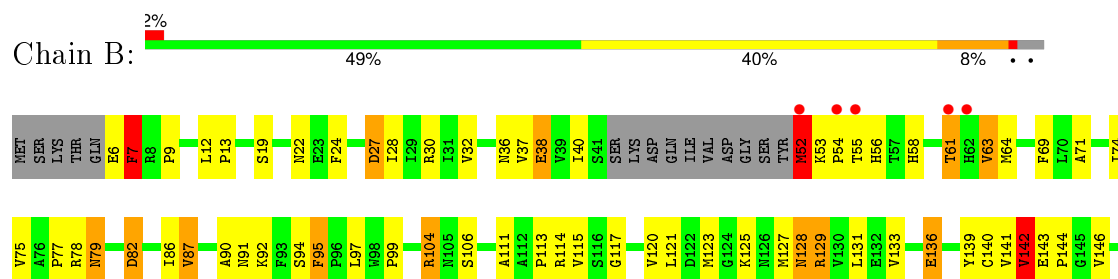
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	129.28Å 129.28Å 130.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.90) 98.1 (19.95-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.312 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.4	EDS
Estimated twinning fraction	0.000 for l,-k,h 0.005 for -l,-k,-h 0.015 for -h,-l,-k 0.000 for -h,l,k 0.039 for -h,k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 23278 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	4/4428 (0.1%)	1.88	123/6018 (2.0%)
1	B	0.80	10/4428 (0.2%)	1.81	92/6018 (1.5%)
All	All	0.78	14/8856 (0.2%)	1.85	215/12036 (1.8%)

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	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	LYS	CG-CD	-24.75	0.68	1.52
1	B	53	LYS	CB-CG	18.00	2.01	1.52
1	B	52	MET	CA-CB	15.90	1.89	1.53
1	B	476	LYS	CG-CD	12.89	1.96	1.52
1	B	325	ARG	CB-CG	-9.83	1.26	1.52
1	B	53	LYS	CA-CB	9.25	1.74	1.53
1	B	221	LYS	CG-CD	-8.71	1.22	1.52
1	B	95	PHE	CB-CG	-6.40	1.40	1.51
1	A	35	GLU	CB-CG	6.11	1.63	1.52
1	A	372	LYS	CG-CD	6.05	1.73	1.52
1	B	52	MET	CB-CG	5.91	1.70	1.51
1	A	66	GLN	CA-CB	-5.24	1.42	1.53
1	B	30	ARG	CB-CG	-5.23	1.38	1.52
1	B	229	LYS	CG-CD	-5.15	1.34	1.52

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	TYR	CB-CG-CD1	21.52	133.91	121.00
1	B	463	ARG	NE-CZ-NH1	20.52	130.56	120.30
1	A	221	LYS	CG-CD-CE	-19.44	53.59	111.90
1	B	325	ARG	CB-CG-CD	19.04	161.11	111.60
1	B	53	LYS	CB-CA-C	18.17	146.73	110.40
1	A	221	LYS	CB-CG-CD	16.95	155.67	111.60
1	B	325	ARG	CA-CB-CG	16.70	150.15	113.40
1	B	211	ARG	CD-NE-CZ	14.89	144.44	123.60
1	A	190	TYR	CB-CG-CD2	-14.55	112.27	121.00
1	A	104	ARG	NE-CZ-NH1	13.93	127.26	120.30
1	A	211	ARG	CD-NE-CZ	13.61	142.65	123.60
1	B	463	ARG	NE-CZ-NH2	-13.53	113.53	120.30
1	B	78	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	B	104	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	B	476	LYS	CB-CG-CD	12.52	144.14	111.60
1	A	129	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	446	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	A	104	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	A	211	ARG	NE-CZ-NH2	-12.34	114.13	120.30
1	B	489	ARG	NE-CZ-NH1	-12.27	114.17	120.30
1	A	78	ARG	NE-CZ-NH1	-12.17	114.21	120.30
1	B	129	ARG	NE-CZ-NH2	-11.47	114.57	120.30
1	A	482	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	B	52	MET	N-CA-CB	10.92	130.26	110.60
1	A	288	ASP	CB-CG-OD2	-10.83	108.55	118.30
1	B	221	LYS	CB-CG-CD	10.78	139.62	111.60
1	A	170	ASP	CB-CG-OD2	10.67	127.90	118.30
1	A	526	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	A	129	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	B	300	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	A	244	TYR	CA-C-N	10.36	136.93	116.20
1	A	446	ARG	NH1-CZ-NH2	10.19	130.61	119.40
1	A	446	ARG	NE-CZ-NH1	-10.05	115.28	120.30
1	A	232	ASP	CB-CG-OD2	9.66	127.00	118.30
1	B	104	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	B	364	ARG	NE-CZ-NH2	9.60	125.10	120.30
1	B	482	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	B	340	ASP	CB-CG-OD1	-9.37	109.87	118.30
1	A	291	GLN	OE1-CD-NE2	9.33	143.36	121.90
1	A	136	GLU	CA-CB-CG	9.28	133.82	113.40
1	A	254	PHE	CB-CG-CD2	9.24	127.27	120.80
1	A	219	ASP	CB-CG-OD1	9.22	126.60	118.30
1	A	254	PHE	CB-CG-CD1	-9.12	114.42	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	ASP	CB-CG-OD1	9.02	126.42	118.30
1	B	291	GLN	OE1-CD-NE2	8.80	142.15	121.90
1	A	435	ASP	CB-CG-OD1	8.80	126.22	118.30
1	A	82	ASP	CB-CG-OD1	8.59	126.03	118.30
1	A	37	VAL	O-C-N	-8.33	109.38	122.70
1	B	211	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	B	244	TYR	CB-CG-CD2	-8.23	116.06	121.00
1	B	170	ASP	CB-CG-OD2	8.21	125.68	118.30
1	B	53	LYS	N-CA-CB	-8.20	95.83	110.60
1	B	232	ASP	CB-CG-OD2	8.16	125.65	118.30
1	B	350	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	B	476	LYS	CG-CD-CE	8.07	136.10	111.90
1	B	325	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	536	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	114	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	B	136	GLU	CA-CB-CG	7.68	130.31	113.40
1	B	446	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	142	VAL	N-CA-CB	-7.65	94.67	111.50
1	A	244	TYR	CB-CG-CD1	7.63	125.58	121.00
1	B	297	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	A	528	ASN	O-C-N	-7.52	110.67	122.70
1	A	249	TYR	CB-CG-CD1	7.51	125.50	121.00
1	B	128	ASN	CB-CA-C	-7.46	95.47	110.40
1	B	190	TYR	CB-CG-CD1	7.36	125.41	121.00
1	A	78	ARG	NH1-CZ-NH2	7.27	127.39	119.40
1	B	297	ARG	CD-NE-CZ	7.22	133.71	123.60
1	A	350	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	353	PHE	CB-CG-CD2	7.20	125.84	120.80
1	A	249	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	A	128	ASN	CB-CA-C	-7.09	96.21	110.40
1	A	222	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	177	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	211	ARG	CG-CD-NE	7.06	126.62	111.80
1	A	526	ARG	NH1-CZ-NH2	-7.06	111.64	119.40
1	A	82	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	B	364	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	211	ARG	NH1-CZ-NH2	6.99	127.08	119.40
1	A	388	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	177	LEU	CA-CB-CG	6.98	131.36	115.30
1	A	387	GLU	OE1-CD-OE2	-6.96	114.95	123.30
1	B	200	MET	CA-CB-CG	6.94	125.09	113.30
1	B	373	ASP	CB-CG-OD1	-6.87	112.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	GLY	CA-C-O	6.84	132.90	120.60
1	A	515	GLU	OE1-CD-OE2	-6.79	115.15	123.30
1	A	463	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	167	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	211	ARG	CA-CB-CG	6.64	128.00	113.40
1	B	457	THR	CB-CA-C	-6.62	93.73	111.60
1	A	465	MET	CA-CB-CG	6.62	124.55	113.30
1	B	211	ARG	N-CA-CB	6.62	122.51	110.60
1	B	211	ARG	CG-CD-NE	6.53	125.52	111.80
1	B	344	LYS	CB-CG-CD	-6.49	94.72	111.60
1	A	59	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	7	PHE	N-CA-C	6.46	128.46	111.00
1	A	361	GLU	CG-CD-OE1	6.43	131.17	118.30
1	B	336	ASP	CB-CG-OD1	-6.43	112.52	118.30
1	A	95	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	A	373	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	A	211	ARG	CA-CB-CG	6.41	127.49	113.40
1	A	338	GLU	OE1-CD-OE2	6.40	130.97	123.30
1	A	244	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	B	453	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	463	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	165	TRP	CA-CB-CG	6.38	125.82	113.70
1	A	511	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	249	TYR	O-C-N	-6.35	112.53	122.70
1	B	304	ALA	CA-C-O	6.31	133.35	120.10
1	A	37	VAL	CA-C-N	6.26	130.96	117.20
1	A	7	PHE	N-CA-C	6.23	127.81	111.00
1	B	291	GLN	CG-CD-OE1	-6.22	109.16	121.60
1	B	365	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	A	139	TYR	CB-CG-CD2	6.14	124.69	121.00
1	B	27	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	B	489	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	A	95	PHE	CB-CG-CD1	6.09	125.06	120.80
1	A	361	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	B	139	TYR	CB-CG-CD2	6.07	124.64	121.00
1	A	36	ASN	CA-C-O	-6.01	107.49	120.10
1	A	137	GLY	CA-C-N	-6.00	103.99	117.20
1	B	182	GLU	CG-CD-OE2	-6.00	106.30	118.30
1	A	150	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	142	VAL	N-CA-CB	-5.95	98.41	111.50
1	A	167	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	294	ASP	CB-CG-OD2	-5.92	112.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	123	MET	CG-SD-CE	-5.91	90.74	100.20
1	A	199	GLY	CA-C-O	-5.89	110.00	120.60
1	A	350	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	244	TYR	CA-C-O	-5.86	107.79	120.10
1	B	92	LYS	CD-CE-NZ	5.83	125.11	111.70
1	B	300	ARG	NH1-CZ-NH2	5.82	125.80	119.40
1	A	246	PHE	CG-CD1-CE1	5.76	127.14	120.80
1	A	37	VAL	CA-C-O	-5.74	108.05	120.10
1	B	82	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	505	THR	CB-CA-C	-5.71	96.18	111.60
1	A	384	TYR	CB-CA-C	-5.68	99.03	110.40
1	A	291	GLN	CG-CD-OE1	-5.68	110.24	121.60
1	B	167	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	301	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	500	TRP	CA-CB-CG	5.67	124.47	113.70
1	A	457	THR	CB-CA-C	-5.65	96.35	111.60
1	A	24	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	B	104	ARG	CD-NE-CZ	5.63	131.48	123.60
1	B	219	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	B	226	MET	CA-CB-CG	5.62	122.86	113.30
1	B	38	GLU	CB-CA-C	-5.59	99.23	110.40
1	A	136	GLU	CG-CD-OE1	5.58	129.47	118.30
1	B	396	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	398	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	182	GLU	CG-CD-OE1	5.54	129.39	118.30
1	A	259	MET	CA-CB-CG	-5.54	103.88	113.30
1	B	261	ILE	CA-CB-CG1	-5.54	100.48	111.00
1	A	90	ALA	CB-CA-C	-5.53	101.80	110.10
1	B	78	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	B	272	ASN	OD1-CG-ND2	5.53	134.61	121.90
1	A	219	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	505	THR	N-CA-CB	5.52	120.79	110.30
1	A	199	GLY	CA-C-N	5.52	129.34	117.20
1	A	349	GLY	CA-C-O	5.51	130.52	120.60
1	A	489	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	465	MET	CA-CB-CG	5.49	122.64	113.30
1	A	130	VAL	N-CA-C	-5.48	96.20	111.00
1	A	560	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	286	ASP	CA-C-N	5.47	127.15	116.20
1	A	242	PHE	CA-CB-CG	5.46	127.01	113.90
1	B	106	SER	CA-C-N	5.45	127.11	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ALA	N-CA-CB	5.45	117.73	110.10
1	A	268	TRP	O-C-N	-5.43	114.02	122.70
1	A	115	VAL	CA-CB-CG2	5.42	119.03	110.90
1	A	36	ASN	CA-C-N	5.41	129.10	117.20
1	B	373	ASP	OD1-CG-OD2	5.41	133.57	123.30
1	A	106	SER	CA-C-N	5.40	126.99	116.20
1	B	384	TYR	CB-CA-C	-5.39	99.62	110.40
1	B	87	VAL	CA-CB-CG1	5.37	118.95	110.90
1	A	504	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	211	ARG	CB-CA-C	-5.35	99.69	110.40
1	B	6	GLU	C-N-CA	5.34	135.06	121.70
1	A	128	ASN	N-CA-C	5.30	125.32	111.00
1	A	61	THR	N-CA-C	-5.29	96.71	111.00
1	B	150	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	82	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	B	184	GLY	CA-C-N	5.23	128.71	117.20
1	A	482	ARG	NH1-CZ-NH2	5.22	125.15	119.40
1	B	303	MET	O-C-N	-5.21	114.36	122.70
1	A	222	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	B	198	SER	O-C-N	5.21	132.06	123.20
1	A	340	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	545	LYS	CB-CA-C	5.21	120.81	110.40
1	B	297	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	A	198	SER	N-CA-C	-5.19	96.99	111.00
1	B	365	ARG	CD-NE-CZ	5.19	130.86	123.60
1	A	511	ASP	OD1-CG-OD2	5.18	133.14	123.30
1	B	482	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	B	203	VAL	CA-C-O	-5.18	109.23	120.10
1	A	118	SER	O-C-N	5.17	130.97	122.70
1	A	24	PHE	N-CA-CB	-5.16	101.32	110.60
1	B	114	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	364	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	542	ALA	N-CA-CB	-5.12	102.93	110.10
1	A	536	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	497	ALA	N-CA-CB	-5.11	102.94	110.10
1	B	485	GLN	OE1-CD-NE2	-5.11	110.16	121.90
1	B	229	LYS	CB-CG-CD	5.09	124.84	111.60
1	A	190	TYR	CG-CD1-CE1	5.08	125.37	121.30
1	A	200	MET	O-C-N	5.08	130.83	122.70
1	A	459	THR	OG1-CB-CG2	-5.06	98.36	110.00
1	A	128	ASN	N-CA-CB	-5.05	101.50	110.60
1	A	421	ALA	N-CA-C	-5.05	97.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	B	453	ASP	OD1-CG-OD2	5.04	132.88	123.30
1	A	259	MET	CA-C-N	5.03	126.27	116.20
1	B	510	MET	CG-SD-CE	5.02	108.23	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	VAL	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	4311	0	4260	210	18
1	B	4311	0	4260	192	10
2	A	12	0	0	2	0
2	B	8	0	0	1	0
All	All	8642	0	8520	364	18

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 22.

All (364) 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:63:VAL:HG11	1:B:423:LEU:HD11	1.44	1.00
1:B:310:THR:HG22	1:B:459:THR:HG22	1.45	0.96
1:A:357:LEU:HB3	1:A:364:ARG:HG2	1.55	0.89
1:A:310:THR:HG22	1:A:459:THR:HG22	1.55	0.88
1:B:79:ASN:ND2	1:B:82:ASP:H	1.74	0.86
1:A:79:ASN:ND2	1:A:82:ASP:H	1.73	0.86
1:A:200:MET:HB3	1:A:265:ILE:HG13	1.56	0.86
1:A:552:GLN:H	1:A:552:GLN:NE2	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG11	1:A:423:LEU:HD11	1.59	0.83
1:B:357:LEU:HB3	1:B:364:ARG:HG2	1.61	0.82
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.60	0.82
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.63	0.80
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.63	0.80
1:B:552:GLN:NE2	1:B:552:GLN:H	1.80	0.79
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.65	0.79
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.13	0.78
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.14	0.78
1:B:40:ILE:HD11	1:B:74:ILE:HD11	1.65	0.77
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.64	0.77
1:A:168:VAL:HG11	1:A:406:PRO:HB3	1.69	0.75
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.69	0.74
1:A:238:ILE:HG21	1:B:428:ILE:HG21	1.70	0.73
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.17	0.72
1:B:280:LEU:HB3	1:B:395:LEU:HD22	1.72	0.72
1:A:310:THR:CG2	1:A:459:THR:HG22	2.20	0.71
1:B:79:ASN:HD21	1:B:82:ASP:H	1.38	0.71
1:A:40:ILE:HD11	1:A:74:ILE:HD11	1.71	0.70
1:B:250:ILE:HD12	1:B:254:PHE:HE2	1.56	0.70
1:A:183:ARG:HD2	1:B:244:TYR:CD2	2.26	0.70
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.73	0.70
1:A:463:ARG:O	1:B:241:LEU:HB3	1.91	0.70
1:A:502:GLU:HB2	1:A:513:ILE:HD13	1.73	0.70
1:A:552:GLN:HE21	1:A:552:GLN:H	1.37	0.69
1:A:319:ALA:HB1	1:A:413:TRP:HB2	1.75	0.68
1:B:290:LYS:HB2	1:B:437:MET:HG3	1.75	0.68
1:A:238:ILE:HG21	1:B:428:ILE:CG2	2.24	0.68
1:B:52:MET:O	1:B:54:PRO:HD3	1.94	0.68
1:A:277:GLN:HB3	1:A:357:LEU:HD12	1.77	0.67
1:A:56:HIS:HA	1:A:111:ALA:HB3	1.76	0.67
1:B:277:GLN:HB3	1:B:357:LEU:HD12	1.76	0.66
1:B:297:ARG:HH11	1:B:298:PRO:HD3	1.60	0.66
1:B:168:VAL:HG11	1:B:406:PRO:HB3	1.78	0.66
1:A:52:MET:O	1:A:54:PRO:HD3	1.96	0.65
1:A:38:GLU:HB3	1:A:74:ILE:CD1	2.27	0.65
1:A:258:ASN:OD1	1:A:532:LYS:HE2	1.97	0.65
1:B:513:ILE:O	1:B:516:THR:HB	1.96	0.65
1:B:275:GLY:HA3	1:B:359:GLY:O	1.95	0.65
1:A:261:ILE:HD11	1:A:541:ILE:HD12	1.79	0.65
1:A:362:PRO:HB2	1:B:366:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HB3	1:A:74:ILE:HD12	1.78	0.65
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.79	0.65
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.28	0.64
1:B:123:MET:O	1:B:127:MET:HB2	1.97	0.64
1:B:427:PRO:HD2	1:B:467:HIS:O	1.98	0.63
1:B:201:GLU:HG3	1:B:211:ARG:HD3	1.80	0.63
1:A:250:ILE:HD12	1:A:254:PHE:HE2	1.63	0.63
1:B:310:THR:CG2	1:B:459:THR:HG22	2.26	0.63
1:A:99:PRO:HA	1:A:121:LEU:HB3	1.81	0.63
1:A:297:ARG:NH1	1:A:298:PRO:HD3	2.13	0.62
1:A:427:PRO:HD2	1:A:467:HIS:O	1.98	0.62
1:B:177:LEU:O	1:B:181:VAL:HG13	1.99	0.62
1:A:315:LEU:HA	1:A:318:ALA:HB3	1.80	0.62
1:B:56:HIS:HA	1:B:111:ALA:HB3	1.81	0.62
1:B:290:LYS:HE3	1:B:294:ASP:OD2	2.00	0.61
1:A:37:VAL:HG13	1:A:75:VAL:HG22	1.82	0.61
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.82	0.61
1:A:79:ASN:HD22	1:A:82:ASP:H	1.48	0.60
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.83	0.60
1:B:297:ARG:NH1	1:B:298:PRO:HD3	2.15	0.60
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.17	0.60
1:A:244:TYR:CD2	1:B:183:ARG:HD2	2.36	0.60
1:A:349:GLY:H	1:A:352:ASN:HD21	1.49	0.60
1:B:289:LEU:HD23	1:B:437:MET:SD	2.41	0.60
1:A:131:LEU:HD12	1:A:141:VAL:HG12	1.84	0.60
1:B:280:LEU:HD12	1:B:281:ILE:N	2.17	0.59
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.17	0.59
1:A:312:ARG:NH2	1:A:410:GLU:OE1	2.35	0.59
1:B:502:GLU:HB2	1:B:513:ILE:HD13	1.85	0.59
1:A:513:ILE:O	1:A:516:THR:HB	2.03	0.59
1:B:183:ARG:NH1	1:B:255:SER:HB3	2.17	0.59
1:B:258:ASN:OD1	1:B:532:LYS:HE2	2.03	0.58
1:B:183:ARG:HH11	1:B:255:SER:HB3	1.68	0.58
1:B:309:PRO:HG2	1:B:460:VAL:HB	1.83	0.58
1:A:183:ARG:NH1	1:A:255:SER:HB3	2.18	0.58
1:B:79:ASN:HD22	1:B:79:ASN:C	2.07	0.58
1:B:200:MET:HB3	1:B:265:ILE:HG13	1.85	0.58
1:A:36:ASN:OD1	1:A:125:LYS:HE2	2.04	0.58
1:A:290:LYS:HE3	1:A:294:ASP:OD2	2.02	0.58
1:B:555:HIS:HB3	1:B:559:LYS:HD2	1.86	0.58
1:A:479:ILE:O	1:A:483:LYS:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLU:HB3	1:B:74:ILE:HD12	1.86	0.57
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.34	0.57
1:A:275:GLY:HA3	1:A:359:GLY:O	2.04	0.57
1:A:91:ASN:OD1	1:A:538:ASN:ND2	2.36	0.57
1:B:91:ASN:OD1	1:B:538:ASN:ND2	2.36	0.57
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.87	0.56
1:B:140:CYS:SG	1:B:269:LEU:HD21	2.45	0.56
1:B:297:ARG:HB3	1:B:297:ARG:HH11	1.71	0.56
1:A:505:THR:OG1	1:A:513:ILE:HD12	2.06	0.56
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.40	0.56
1:B:261:ILE:HD11	1:B:541:ILE:HD12	1.88	0.56
1:B:69:PHE:O	1:B:113:PRO:HD2	2.05	0.56
1:A:183:ARG:HH11	1:A:255:SER:HB3	1.71	0.56
1:A:54:PRO:HG3	1:A:104:ARG:HG3	1.89	0.55
1:B:36:ASN:OD1	1:B:125:LYS:HE2	2.06	0.55
1:B:258:ASN:CG	1:B:532:LYS:HE2	2.27	0.55
1:B:7:PHE:HA	1:B:22:ASN:OD1	2.07	0.55
1:A:443:THR:HA	1:A:491:LEU:HD21	1.89	0.55
1:A:79:ASN:HD21	1:A:82:ASP:H	1.53	0.55
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.20	0.55
1:B:63:VAL:CG1	1:B:423:LEU:HD11	2.27	0.55
1:B:75:VAL:HG11	1:B:86:ILE:HD13	1.89	0.55
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.42	0.55
1:A:420:GLY:HA2	1:A:473:PHE:O	2.06	0.54
1:A:284:PRO:HD2	1:A:288:ASP:OD2	2.07	0.54
1:A:75:VAL:HG11	1:A:86:ILE:HD13	1.88	0.54
1:B:99:PRO:HA	1:B:121:LEU:HB3	1.89	0.54
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.35	0.54
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.43	0.54
1:A:257:SER:HB2	1:B:248:PRO:HG3	1.90	0.54
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.37	0.53
1:A:290:LYS:HB2	1:A:437:MET:HG3	1.89	0.53
1:A:194:TRP:O	1:A:197:HIS:HD2	1.91	0.53
1:A:309:PRO:HD2	1:A:460:VAL:HB	1.88	0.53
1:B:194:TRP:O	1:B:197:HIS:HD2	1.91	0.53
1:B:332:GLU:HB3	1:B:333:PRO:CD	2.37	0.53
1:A:280:LEU:HD12	1:A:281:ILE:N	2.23	0.53
1:A:315:LEU:HD22	1:A:416:TRP:CH2	2.44	0.53
1:A:488:MET:HG2	1:A:509:PHE:CE2	2.44	0.52
1:B:54:PRO:HG3	1:B:104:ARG:HG3	1.90	0.52
1:B:38:GLU:HB3	1:B:74:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:PRO:HG2	1:B:460:VAL:CG2	2.39	0.52
1:B:64:MET:SD	1:B:485:GLN:OE1	2.67	0.52
1:B:443:THR:HA	1:B:491:LEU:HD21	1.90	0.52
1:A:31:ILE:HD13	1:A:85:SER:HB3	1.92	0.52
1:A:241:LEU:HB3	1:B:463:ARG:O	2.09	0.52
1:B:312:ARG:NH2	1:B:410:GLU:OE1	2.43	0.52
1:A:38:GLU:O	1:A:73:ALA:HA	2.10	0.52
1:B:332:GLU:CB	1:B:333:PRO:HD2	2.38	0.52
1:A:297:ARG:HH11	1:A:298:PRO:HD3	1.75	0.52
1:A:195:MET:SD	1:B:195:MET:SD	3.08	0.52
1:A:237:LYS:HD2	1:B:500:TRP:CD1	2.45	0.52
1:A:332:GLU:CB	1:A:333:PRO:HD2	2.37	0.51
1:A:142:VAL:HG22	1:A:146:VAL:CG2	2.38	0.51
1:A:257:SER:CB	1:B:248:PRO:HG3	2.41	0.51
1:A:280:LEU:HB3	1:A:395:LEU:HD22	1.92	0.51
1:B:505:THR:OG1	1:B:513:ILE:HD12	2.11	0.51
1:A:473:PHE:CG	1:A:484:VAL:HG21	2.46	0.51
1:B:387:GLU:HA	1:B:396:ARG:NH2	2.26	0.51
1:A:183:ARG:HD2	1:B:244:TYR:CE2	2.46	0.51
1:A:79:ASN:HD22	1:A:79:ASN:C	2.15	0.50
1:A:31:ILE:HD13	1:A:85:SER:CB	2.41	0.50
1:A:550:PRO:HG2	1:A:553:TYR:HD1	1.77	0.50
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.27	0.50
1:A:426:SER:O	1:A:502:GLU:HA	2.12	0.50
1:A:253:LEU:CG	1:B:253:LEU:HD21	2.41	0.50
1:A:280:LEU:CB	1:A:395:LEU:HD22	2.42	0.50
1:A:494:ASP:O	1:A:497:ALA:HB3	2.11	0.50
1:B:55:THR:HG21	1:B:58:HIS:CE1	2.46	0.50
1:B:552:GLN:HE21	1:B:552:GLN:H	1.52	0.50
1:B:319:ALA:HB1	1:B:413:TRP:HB2	1.93	0.50
1:A:366:VAL:HG21	1:B:362:PRO:HB2	1.93	0.50
1:A:229:LYS:O	1:A:233:GLN:HG3	2.12	0.50
1:A:63:VAL:HG12	1:A:473:PHE:CZ	2.46	0.50
1:A:24:PHE:O	1:A:27:ASP:HB2	2.12	0.50
1:A:271:PRO:O	1:A:272:ASN:C	2.50	0.50
1:A:413:TRP:CH2	1:A:470:CYS:HB3	2.47	0.49
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.47	0.49
1:A:179:ASN:OD1	1:A:193:HIS:ND1	2.43	0.49
1:A:480:GLN:O	1:A:483:LYS:HB2	2.12	0.49
1:B:488:MET:HG2	1:B:509:PHE:CE2	2.47	0.49
1:B:315:LEU:HD22	1:B:416:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ASP:N	1:A:537:PRO:CD	2.76	0.49
1:B:199:GLY:HA3	1:B:240:HIS:CD2	2.48	0.49
1:A:69:PHE:O	1:A:113:PRO:HD2	2.13	0.49
1:A:37:VAL:HG13	1:A:75:VAL:CG2	2.42	0.49
1:A:369:GLU:O	1:A:373:ASP:HB2	2.12	0.49
1:A:363:ILE:HD13	1:B:363:ILE:HG23	1.94	0.49
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.48	0.49
1:B:309:PRO:HG2	1:B:460:VAL:CB	2.42	0.48
1:A:197:HIS:HA	1:A:266:GLY:O	2.14	0.48
1:B:230:PRO:HA	1:B:233:GLN:CD	2.33	0.48
1:A:74:ILE:HG23	1:A:120:VAL:HG12	1.96	0.48
1:A:312:ARG:HD3	1:A:317:ASP:OD1	2.14	0.48
1:A:177:LEU:O	1:A:181:VAL:HG13	2.13	0.48
1:B:479:ILE:O	1:B:483:LYS:HG3	2.12	0.48
1:B:511:ASP:O	1:B:512:GLN:C	2.50	0.48
1:A:201:GLU:HB3	1:A:264:LYS:HB2	1.96	0.48
1:A:7:PHE:HA	1:A:22:ASN:OD1	2.13	0.48
1:A:319:ALA:CB	1:A:413:TRP:HB2	2.42	0.48
1:B:40:ILE:HD11	1:B:74:ILE:CD1	2.40	0.48
1:B:187:TYR:O	1:B:402:MET:HG2	2.14	0.48
1:A:332:GLU:HB3	1:A:333:PRO:CD	2.39	0.48
1:A:253:LEU:HD21	1:B:253:LEU:CG	2.44	0.48
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.49	0.48
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.48	0.48
1:A:289:LEU:HD23	1:A:437:MET:SD	2.54	0.47
1:B:354:TYR:CE2	1:B:394:VAL:HG12	2.49	0.47
1:A:32:VAL:HG12	1:A:82:ASP:OD2	2.14	0.47
1:B:443:THR:HG21	1:B:469:VAL:CG2	2.44	0.47
1:A:217:LEU:HD13	1:A:217:LEU:C	2.35	0.47
1:A:363:ILE:CD1	1:B:363:ILE:HG23	2.43	0.47
1:A:248:PRO:HG3	1:B:257:SER:HB2	1.96	0.47
1:B:229:LYS:O	1:B:233:GLN:HG3	2.14	0.47
1:A:387:GLU:HA	1:A:396:ARG:NH2	2.29	0.47
1:B:71:ALA:HB2	1:B:120:VAL:HG23	1.96	0.47
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.15	0.47
1:B:492:ILE:HG23	1:B:502:GLU:OE2	2.14	0.47
1:A:363:ILE:HG23	1:B:363:ILE:HD13	1.97	0.47
1:A:77:PRO:O	1:A:126:ASN:HB2	2.14	0.47
1:A:463:ARG:NH2	1:B:269:LEU:O	2.48	0.47
1:B:403:GLN:HG3	1:B:405:ILE:HG13	1.96	0.47
1:A:448:GLN:O	1:A:449:GLU:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:THR:OG1	1:B:421:ALA:HB1	2.14	0.47
1:A:534:ALA:HB1	1:B:530:VAL:HG12	1.97	0.47
1:A:210:LEU:HD11	1:B:524:PHE:HA	1.97	0.47
1:A:258:ASN:CG	1:A:532:LYS:HE2	2.35	0.46
1:B:197:HIS:HA	1:B:266:GLY:O	2.15	0.46
1:B:398:ARG:NH1	1:B:410:GLU:OE2	2.48	0.46
1:B:61:THR:HA	1:B:421:ALA:HB1	1.98	0.46
1:A:286:ASP:HB2	1:A:350:ARG:HG2	1.97	0.46
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.51	0.46
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.81	0.46
1:A:264:LYS:HG3	2:A:2008:HOH:O	2.16	0.46
1:B:378:ILE:O	1:B:381:VAL:HB	2.16	0.46
1:B:131:LEU:HD12	1:B:141:VAL:HG12	1.97	0.46
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.99	0.45
1:B:97:LEU:HD12	1:B:541:ILE:HD13	1.98	0.45
1:A:237:LYS:HD2	1:B:500:TRP:NE1	2.32	0.45
1:A:167:ASP:OD1	1:A:193:HIS:NE2	2.49	0.45
1:A:372:LYS:HG2	1:A:383:PHE:CZ	2.51	0.45
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.51	0.45
1:A:534:ALA:HB2	1:B:534:ALA:HB2	1.97	0.45
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.51	0.45
1:A:443:THR:O	1:A:443:THR:HG22	2.17	0.45
1:B:520:ASN:O	1:B:521:ASN:HB2	2.15	0.45
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.97	0.45
1:A:253:LEU:CD2	1:B:253:LEU:HD21	2.47	0.45
1:B:230:PRO:HA	1:B:233:GLN:NE2	2.32	0.45
1:A:315:LEU:HD22	1:A:416:TRP:CZ2	2.51	0.45
1:B:413:TRP:CH2	1:B:470:CYS:HB3	2.52	0.45
1:A:61:THR:OG1	1:A:421:ALA:HB1	2.16	0.45
1:B:168:VAL:HB	1:B:169:PRO:HD2	1.99	0.45
1:B:224:GLU:H	1:B:224:GLU:CD	2.20	0.45
1:B:559:LYS:HE2	2:B:2007:HOH:O	2.15	0.45
1:A:309:PRO:HG2	1:A:460:VAL:HB	1.99	0.45
1:B:258:ASN:HB2	1:B:541:ILE:O	2.17	0.44
1:A:142:VAL:HG22	1:A:146:VAL:CB	2.48	0.44
1:A:244:TYR:CG	1:B:183:ARG:HD2	2.52	0.44
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.52	0.44
1:A:61:THR:HA	1:A:421:ALA:HB1	1.99	0.44
1:B:549:TRP:HA	1:B:550:PRO:HD3	1.85	0.44
1:A:38:GLU:HB3	1:A:74:ILE:HD13	1.99	0.44
1:B:63:VAL:HG11	1:B:423:LEU:CD1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD21	1:B:253:LEU:CD2	2.47	0.44
1:A:378:ILE:O	1:A:381:VAL:HB	2.18	0.44
1:A:137:GLY:O	1:A:138:ALA:HB3	2.17	0.44
1:A:428:ILE:HG21	1:B:238:ILE:HG21	1.99	0.44
1:B:295:ILE:O	1:B:298:PRO:HD2	2.18	0.44
1:A:211:ARG:HD2	1:A:235:TRP:CH2	2.53	0.44
1:A:144:PRO:HD3	1:A:263:THR:O	2.18	0.44
1:A:553:TYR:HD2	1:A:558:TRP:NE1	2.16	0.43
1:B:349:GLY:H	1:B:352:ASN:HD21	1.65	0.43
1:A:280:LEU:HD12	1:A:280:LEU:C	2.38	0.43
1:B:480:GLN:O	1:B:483:LYS:HB2	2.17	0.43
1:A:346:LEU:O	1:A:347:ASN:HB2	2.18	0.43
1:A:301:LEU:HD22	2:A:2010:HOH:O	2.17	0.43
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.18	0.43
1:A:84:GLN:NE2	1:A:207:GLY:O	2.32	0.43
1:A:473:PHE:CE2	1:A:484:VAL:HG11	2.53	0.43
1:B:386:PRO:HD2	1:B:387:GLU:OE2	2.17	0.43
1:A:372:LYS:HG2	1:A:383:PHE:CE2	2.53	0.43
1:B:308:VAL:HG13	1:B:460:VAL:O	2.18	0.43
1:A:112:ALA:O	1:A:507:LEU:HD11	2.19	0.43
1:B:28:ILE:O	1:B:32:VAL:HG22	2.18	0.43
1:A:505:THR:HG21	1:A:509:PHE:HB2	2.01	0.43
1:A:271:PRO:HG3	1:B:301:LEU:HB3	2.01	0.43
1:B:321:LEU:HD13	1:B:346:LEU:HD22	2.01	0.43
1:B:79:ASN:HD22	1:B:82:ASP:H	1.63	0.43
1:A:131:LEU:HD11	1:A:264:LYS:HG2	2.01	0.43
1:A:307:ASN:O	1:A:309:PRO:HD3	2.19	0.43
1:B:527:PHE:CZ	1:B:531:LEU:HD11	2.54	0.43
1:A:253:LEU:HD21	1:B:253:LEU:HG	2.00	0.43
1:A:9:PRO:HG2	1:A:12:LEU:HD23	2.00	0.43
1:A:78:ARG:HD2	1:A:78:ARG:HH11	1.52	0.42
1:B:201:GLU:HB3	1:B:264:LYS:HB2	2.00	0.42
1:B:526:ARG:HH21	1:B:529:GLU:CD	2.21	0.42
1:A:205:ALA:HB2	1:A:541:ILE:HG12	2.00	0.42
1:A:545:LYS:HD2	1:A:546:SER:N	2.34	0.42
1:A:553:TYR:O	1:A:554:SER:C	2.57	0.42
1:B:417:LEU:HD12	1:B:473:PHE:HA	2.01	0.42
1:A:403:GLN:HG3	1:A:405:ILE:HG13	2.01	0.42
1:A:140:CYS:SG	1:A:269:LEU:HD21	2.59	0.42
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.99	0.42
1:B:387:GLU:HA	1:B:396:ARG:HH22	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:C	1:B:217:LEU:CD1	2.88	0.42
1:B:309:PRO:HD2	1:B:460:VAL:HB	2.00	0.42
1:A:506:HIS:O	1:A:507:LEU:C	2.56	0.42
1:B:206:ASN:OD1	1:B:208:GLU:HB2	2.19	0.42
1:B:340:ASP:O	1:B:343:ALA:HB3	2.19	0.42
1:A:289:LEU:O	1:A:293:VAL:HG23	2.20	0.42
1:A:209:LEU:HD13	1:B:519:TRP:HH2	1.85	0.42
1:B:518:ASN:O	1:B:519:TRP:C	2.56	0.42
1:B:143:GLU:HB3	1:B:144:PRO:CD	2.50	0.42
1:A:372:LYS:HA	1:A:383:PHE:CE1	2.55	0.42
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.19	0.42
1:A:502:GLU:CB	1:A:513:ILE:HD13	2.46	0.42
1:B:315:LEU:HA	1:B:318:ALA:HB3	2.01	0.42
1:B:372:LYS:HG2	1:B:383:PHE:CE2	2.55	0.42
1:B:90:ALA:O	1:B:94:SER:N	2.53	0.42
1:A:28:ILE:O	1:A:32:VAL:HG22	2.20	0.42
1:A:217:LEU:C	1:A:217:LEU:CD1	2.88	0.42
1:A:415:ASP:O	1:A:416:TRP:C	2.58	0.42
1:B:9:PRO:HG2	1:B:12:LEU:CD2	2.50	0.42
1:A:63:VAL:CG1	1:A:423:LEU:HD11	2.40	0.41
1:A:473:PHE:CD2	1:A:484:VAL:HG21	2.55	0.41
1:A:258:ASN:HB2	1:A:542:ALA:HB3	2.02	0.41
1:B:315:LEU:HD22	1:B:416:TRP:CZ2	2.55	0.41
1:B:129:ARG:NH2	1:B:143:GLU:OE2	2.36	0.41
1:A:364:ARG:HD2	1:A:364:ARG:HH11	1.59	0.41
1:A:87:VAL:HG11	1:A:207:GLY:HA2	2.01	0.41
1:B:189:PRO:HB2	1:B:270:MET:HE3	2.02	0.41
1:B:284:PRO:HD2	1:B:288:ASP:OD2	2.20	0.41
1:A:25:ILE:HG22	1:A:29:ILE:HD12	2.02	0.41
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.54	0.41
1:A:321:LEU:HD13	1:A:346:LEU:HD22	2.02	0.41
1:B:231:GLU:H	1:B:231:GLU:HG3	1.15	0.41
1:B:250:ILE:HD12	1:B:254:PHE:CE2	2.46	0.41
1:B:473:PHE:CD2	1:B:484:VAL:HG21	2.55	0.41
1:A:256:GLN:NE2	1:A:504:ARG:HG3	2.34	0.41
1:B:201:GLU:CB	1:B:264:LYS:HB2	2.50	0.41
1:A:250:ILE:HD12	1:A:254:PHE:CE2	2.51	0.41
1:A:309:PRO:HB2	1:A:353:PHE:CZ	2.56	0.41
1:B:90:ALA:HB1	1:B:95:PHE:O	2.20	0.41
1:B:525:LEU:CD1	1:B:548:VAL:HG22	2.50	0.41
1:A:38:GLU:N	1:A:74:ILE:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:O	1:A:319:ALA:HB3	2.20	0.41
1:B:481:LYS:O	1:B:484:VAL:HB	2.21	0.41
1:B:9:PRO:HG2	1:B:12:LEU:HD23	2.02	0.41
1:B:24:PHE:O	1:B:27:ASP:HB2	2.20	0.41
1:B:506:HIS:O	1:B:507:LEU:C	2.59	0.41
1:A:148:TYR:CD1	1:A:168:VAL:HG12	2.56	0.41
1:A:297:ARG:HB3	1:A:297:ARG:HH11	1.86	0.41
1:B:519:TRP:O	1:B:520:ASN:C	2.59	0.41
1:A:105:ASN:O	1:A:106:SER:C	2.58	0.41
1:B:87:VAL:HG11	1:B:207:GLY:HA2	2.02	0.41
1:B:177:LEU:HB2	1:B:265:ILE:CG2	2.51	0.41
1:B:13:PRO:HA	1:B:117:GLY:HA3	2.03	0.41
1:A:255:SER:O	1:A:256:GLN:C	2.59	0.40
1:B:217:LEU:C	1:B:217:LEU:HD13	2.42	0.40
1:A:319:ALA:HB1	1:A:413:TRP:CB	2.49	0.40
1:A:82:ASP:O	1:A:86:ILE:HG13	2.20	0.40
1:A:361:GLU:O	1:A:362:PRO:C	2.60	0.40
1:A:417:LEU:HD12	1:A:473:PHE:HA	2.03	0.40
1:B:309:PRO:O	1:B:460:VAL:HG23	2.22	0.40
1:A:428:ILE:CG2	1:B:238:ILE:HG21	2.51	0.40
1:A:540:ILE:H	1:A:540:ILE:HG13	1.73	0.40
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.57	0.40
1:B:177:LEU:HD12	1:B:177:LEU:C	2.42	0.40
1:B:177:LEU:HB2	1:B:265:ILE:HG21	2.03	0.40
1:B:37:VAL:HG13	1:B:75:VAL:HG22	2.03	0.40
1:A:9:PRO:HG2	1:A:12:LEU:CD2	2.52	0.40
1:B:133:VAL:HG21	1:B:154:TYR:CE1	2.56	0.40
1:B:431:VAL:HG22	1:B:465:MET:CG	2.52	0.40

All (18) 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)
1:A:330:ARG:NH2	1:A:332:GLU:CB[2_765]	0.47	1.73
1:A:52:MET:SD	1:B:415:ASP:OD1[6_655]	0.77	1.43
1:A:18:LEU:CD2	1:A:30:ARG:NH1[3_655]	1.13	1.07
1:A:330:ARG:NH2	1:A:332:GLU:CA[2_765]	1.17	1.03
1:A:53:LYS:CA	1:B:412:LYS:NZ[6_655]	1.35	0.85
1:A:52:MET:SD	1:B:415:ASP:CG[6_655]	1.37	0.83
1:A:330:ARG:CZ	1:A:332:GLU:CB[2_765]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:CE	1:B:415:ASP:CB[6_655]	1.84	0.36
1:A:52:MET:CE	1:B:415:ASP:CG[6_655]	1.84	0.36
1:A:330:ARG:NH2	1:A:332:GLU:CG[2_765]	1.92	0.28
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	1.96	0.24
1:A:52:MET:CE	1:B:415:ASP:OD1[6_655]	2.01	0.19
1:A:52:MET:SD	1:B:415:ASP:OD2[6_655]	2.08	0.12
1:A:330:ARG:NH2	1:A:332:GLU:N[2_765]	2.10	0.10
1:A:337:GLU:OE2	1:A:448:GLN:O[2_765]	2.11	0.09
1:A:330:ARG:NH2	1:A:332:GLU:C[2_765]	2.13	0.07
1:A:53:LYS:C	1:B:412:LYS:NZ[6_655]	2.14	0.06
1:A:373:ASP:OD2	1:B:288:ASP:OD1[4_665]	2.19	0.01

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	541/560 (97%)	494 (91%)	40 (7%)	7 (1%)	15	46
1	B	541/560 (97%)	490 (91%)	47 (9%)	4 (1%)	26	63
All	All	1082/1120 (97%)	984 (91%)	87 (8%)	11 (1%)	19	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	PHE
1	A	7	PHE
1	A	67	ASP
1	B	410	GLU
1	A	410	GLU
1	B	409	ASP
1	A	297	ARG
1	A	409	ASP
1	A	146	VAL

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Mol	Chain	Res	Type
1	A	63	VAL
1	B	63	VAL

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	466/481 (97%)	422 (91%)	44 (9%)	11	32
1	B	466/481 (97%)	423 (91%)	43 (9%)	11	33
All	All	932/962 (97%)	845 (91%)	87 (9%)	11	32

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	61	THR
1	A	79	ASN
1	A	95	PHE
1	A	106	SER
1	A	116	SER
1	A	128	ASN
1	A	136	GLU
1	A	142	VAL
1	A	155	LEU
1	A	177	LEU
1	A	211	ARG
1	A	217	LEU
1	A	220	PRO
1	A	221	LYS
1	A	231	GLU
1	A	237	LYS
1	A	251	ASP
1	A	267	ILE
1	A	290	LYS
1	A	297	ARG

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Mol	Chain	Res	Type
1	A	301	LEU
1	A	303	MET
1	A	323	ASP
1	A	329	SER
1	A	331	THR
1	A	336	ASP
1	A	342	ILE
1	A	350	ARG
1	A	372	LYS
1	A	381	VAL
1	A	387	GLU
1	A	391	GLU
1	A	411	LEU
1	A	432	SER
1	A	446	ARG
1	A	457	THR
1	A	502	GLU
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	532	LYS
1	A	552	GLN
1	A	555	HIS
1	B	19	SER
1	B	52	MET
1	B	61	THR
1	B	77	PRO
1	B	79	ASN
1	B	115	VAL
1	B	128	ASN
1	B	136	GLU
1	B	142	VAL
1	B	155	LEU
1	B	177	LEU
1	B	217	LEU
1	B	231	GLU
1	B	237	LYS
1	B	238	ILE
1	B	267	ILE
1	B	271	PRO
1	B	283	LEU
1	B	297	ARG

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Mol	Chain	Res	Type
1	B	301	LEU
1	B	303	MET
1	B	325	ARG
1	B	329	SER
1	B	331	THR
1	B	336	ASP
1	B	344	LYS
1	B	372	LYS
1	B	381	VAL
1	B	387	GLU
1	B	391	GLU
1	B	411	LEU
1	B	426	SER
1	B	432	SER
1	B	457	THR
1	B	462	MET
1	B	502	GLU
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	523	SER
1	B	551	SER
1	B	552	GLN
1	B	555	HIS

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

Mol	Chain	Res	Type
1	A	62	HIS
1	A	79	ASN
1	A	128	ASN
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	439	GLN
1	A	467	HIS
1	A	520	ASN
1	A	552	GLN
1	B	62	HIS
1	B	79	ASN
1	B	91	ASN
1	B	128	ASN

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Mol	Chain	Res	Type
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	467	HIS
1	B	520	ASN
1	B	538	ASN
1	B	552	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	545/560 (97%)	-0.31	6 (1%) 82 80	3, 14, 38, 49	30 (5%)
1	B	545/560 (97%)	-0.27	9 (1%) 73 70	3, 14, 38, 50	30 (5%)
All	All	1090/1120 (97%)	-0.29	15 (1%) 78 76	3, 14, 38, 50	60 (5%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	MET	4.3
1	A	409	ASP	3.9
1	B	55	THR	3.1
1	B	418	PRO	3.1
1	B	409	ASP	3.1
1	B	411	LEU	2.6
1	B	54	PRO	2.3
1	A	62	HIS	2.3
1	B	61	THR	2.3
1	A	104	ARG	2.3
1	B	62	HIS	2.1
1	A	325	ARG	2.1
1	A	6	GLU	2.1
1	A	10	LEU	2.1
1	B	410	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.