



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:09 AM UTC

PDB ID : 6XF9 / pdb_00006xf9
Title : Crystal structure of KSHV ORF68
Authors : Didychuk, A.L.; Gates, S.N.; Martin, A.; Glaunsinger, B.
Deposited on : 2020-06-15
Resolution : 2.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

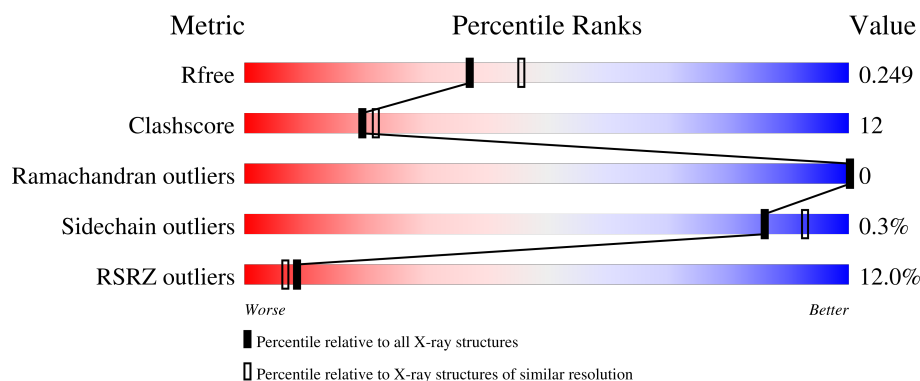
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	467	8% 70% 20% 9%
1	B	467	9% 72% 17% 9%
1	C	467	10% 71% 19% 9%
1	D	467	11% 76% 15% 9%
1	E	467	16% 71% 19% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16391 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 Packaging protein UL32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3284	2106	555	594	29			
1	B	424	Total	C	N	O	S	0	1	0
			3262	2093	554	587	28			
1	C	424	Total	C	N	O	S	0	1	0
			3277	2104	555	589	29			
1	D	426	Total	C	N	O	S	0	1	0
			3283	2106	556	592	29			
1	E	425	Total	C	N	O	S	0	0	0
			3267	2095	550	593	29			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		
2	C	3	Total	Zn	0	0
			3	3		
2	D	3	Total	Zn	0	0
			3	3		
2	E	3	Total	Zn	0	0
			3	3		

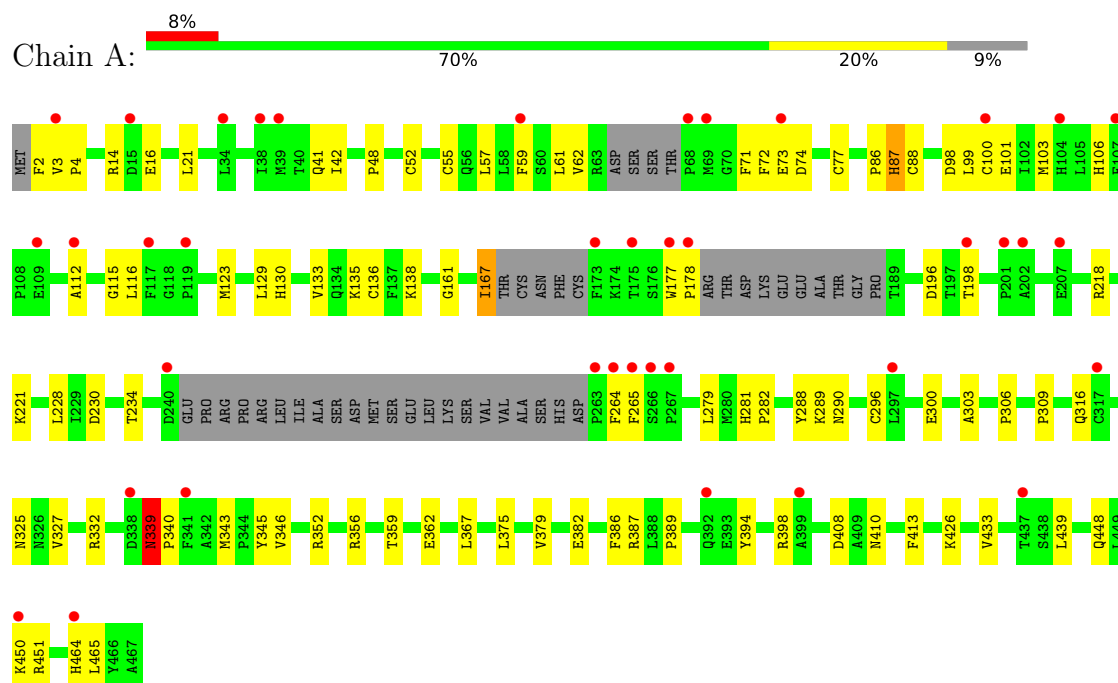
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	D	2	Total	O	0	0
			2	2		

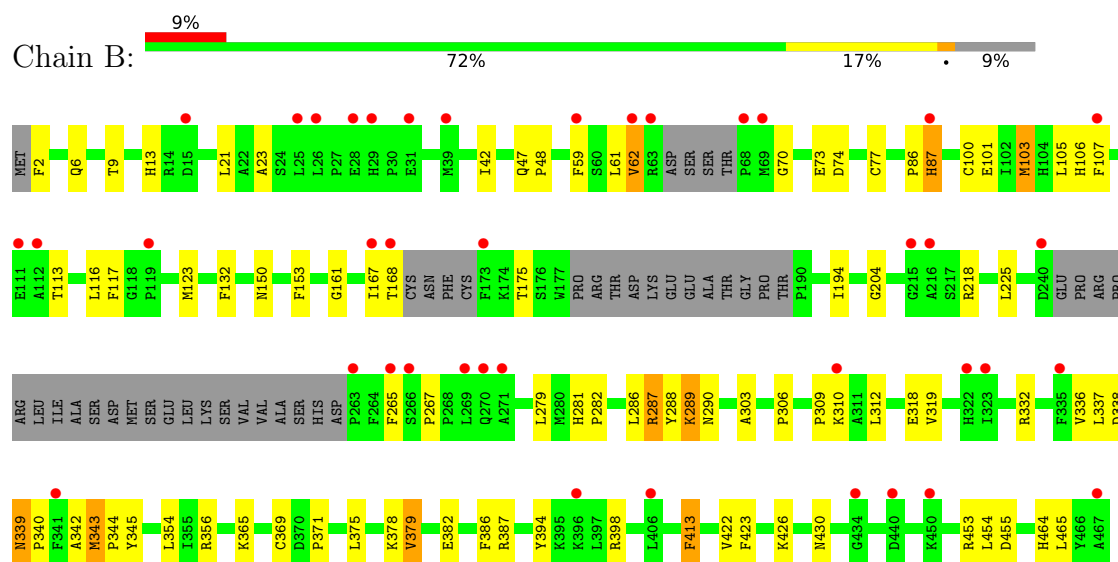
3 Residue-property plots [i](#)

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.

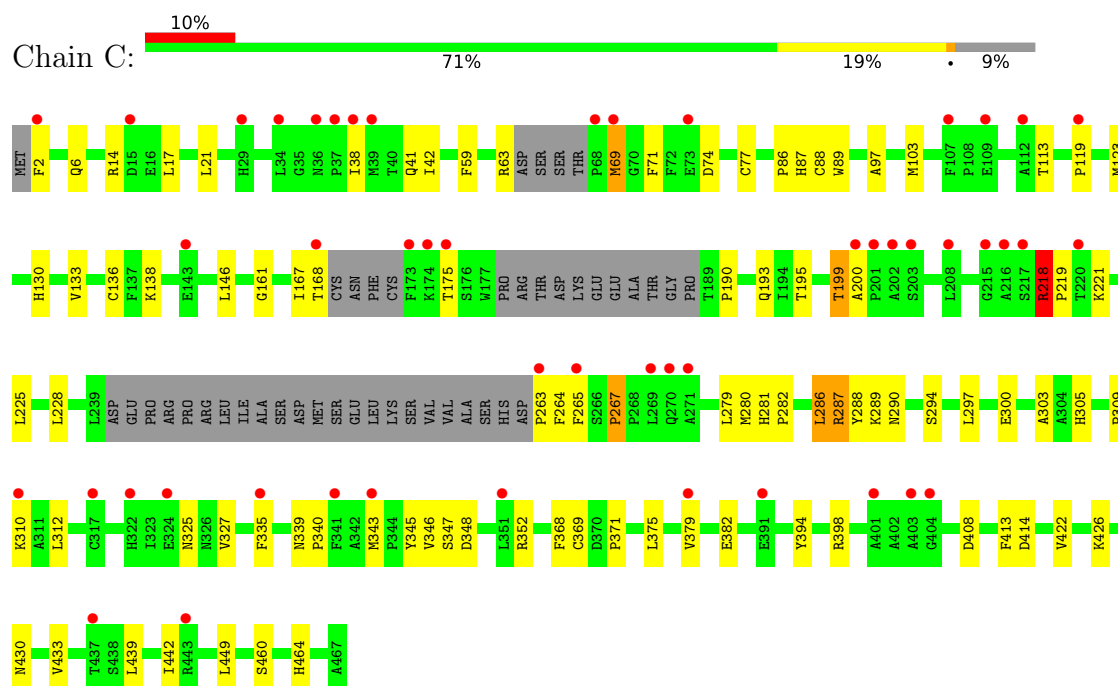
• Molecule 1: Packaging protein UL32



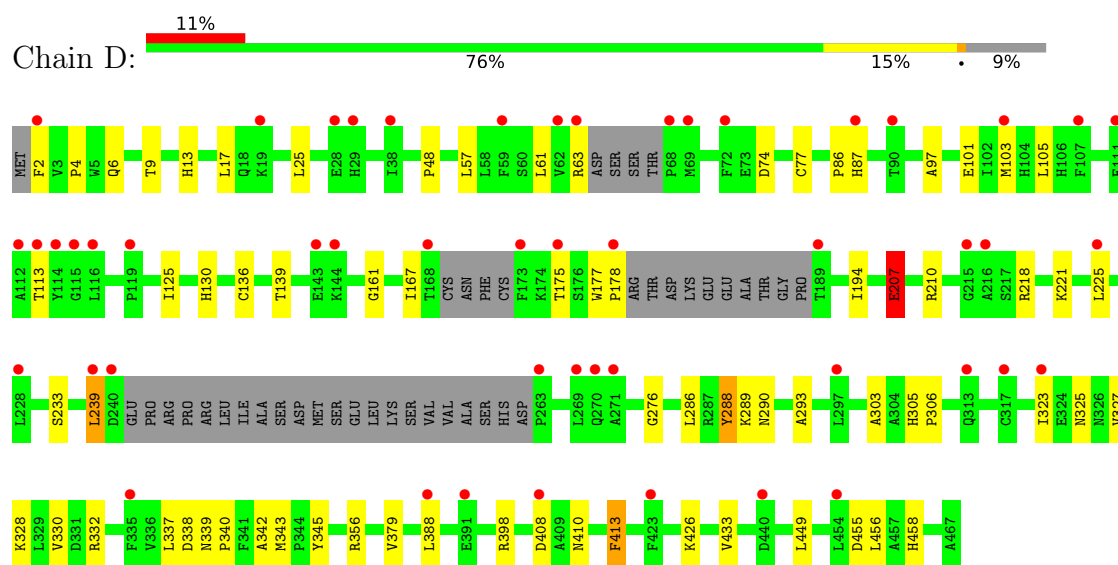
• Molecule 1: Packaging protein UL32



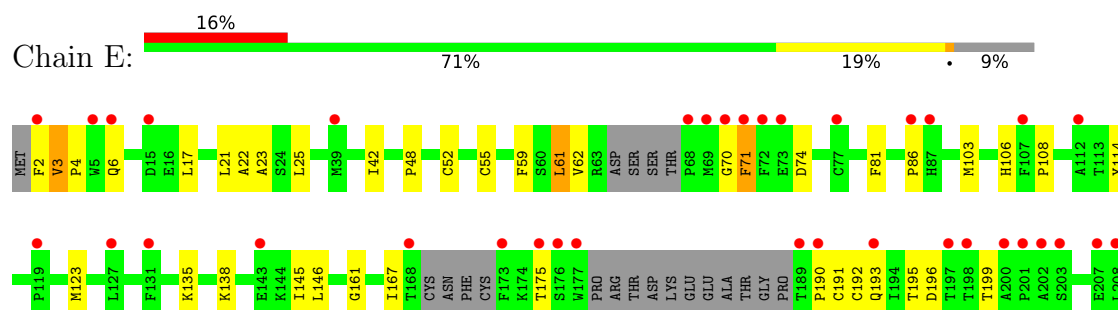
• Molecule 1: Packaging protein UL32

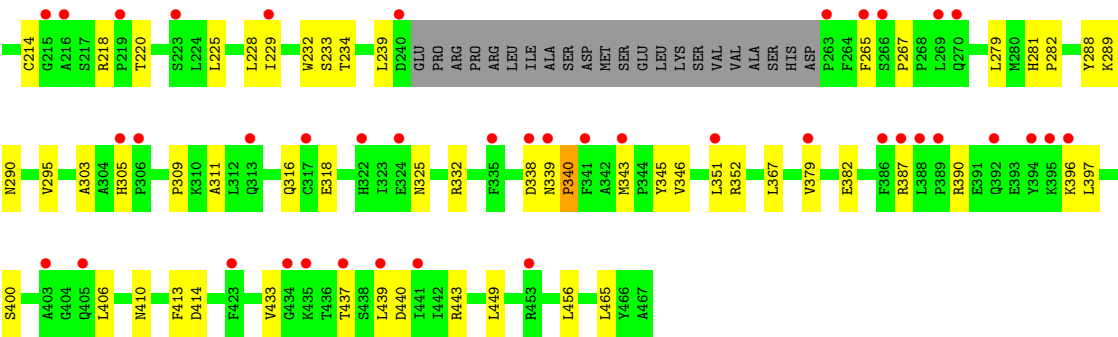


• Molecule 1: Packaging protein UL32



• Molecule 1: Packaging protein UL32





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.99Å 224.04Å 192.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 2.22 49.54 – 2.22	Depositor EDS
% Data completeness (in resolution range)	63.4 (49.54-2.22) 65.1 (49.54-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.222 , 0.248 0.224 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.013 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16391	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.83	12/3367 (0.4%)	0.85	10/4578 (0.2%)
1	B	0.79	11/3344 (0.3%)	0.87	16/4547 (0.4%)
1	C	0.78	6/3357 (0.2%)	0.87	14/4564 (0.3%)
1	D	0.72	8/3366 (0.2%)	0.75	7/4578 (0.2%)
1	E	0.70	5/3345 (0.1%)	0.77	6/4549 (0.1%)
All	All	0.77	42/16779 (0.3%)	0.82	53/22816 (0.2%)

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
1	E	0	1
All	All	0	2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	340	PRO	N-CD	16.05	1.70	1.47
1	A	99	LEU	C-N	11.20	1.48	1.33
1	A	87[A]	HIS	CA-C	9.19	1.64	1.52
1	A	87[B]	HIS	CA-C	9.19	1.64	1.52
1	D	87[A]	HIS	CA-C	8.89	1.64	1.52
1	D	87[B]	HIS	CA-C	8.89	1.64	1.52
1	B	87[A]	HIS	CA-C	8.59	1.63	1.52
1	B	87[B]	HIS	CA-C	8.59	1.63	1.52
1	A	100	CYS	N-CA	7.94	1.55	1.46
1	A	100	CYS	C-N	-7.93	1.23	1.33
1	A	290	ASN	C-O	-7.34	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	290	ASN	C-O	-7.27	1.14	1.23
1	A	98	ASP	C-N	7.19	1.43	1.33
1	A	288	TYR	C-O	-6.88	1.15	1.24
1	C	290	ASN	C-O	-6.85	1.14	1.23
1	B	289	LYS	C-O	-6.79	1.15	1.23
1	A	288	TYR	CA-C	-6.69	1.44	1.52
1	A	101	GLU	C-O	-6.55	1.16	1.24
1	A	100	CYS	C-O	6.53	1.31	1.24
1	D	289	LYS	C-O	-6.51	1.15	1.23
1	A	413	PHE	C-O	-6.50	1.15	1.23
1	C	288	TYR	CA-C	-6.49	1.44	1.52
1	B	290	ASN	C-O	-6.34	1.15	1.23
1	E	289	LYS	C-O	-6.32	1.16	1.23
1	D	207	GLU	C-O	-6.30	1.16	1.24
1	B	288	TYR	C-O	-6.17	1.16	1.24
1	B	455	ASP	CA-C	-6.11	1.45	1.52
1	B	413	PHE	C-O	-6.02	1.16	1.23
1	B	378	LYS	C-O	-5.90	1.17	1.24
1	C	267	PRO	C-O	-5.86	1.18	1.24
1	B	286	LEU	C-O	-5.76	1.17	1.24
1	B	288	TYR	CA-C	-5.60	1.45	1.52
1	E	413	PHE	C-O	-5.59	1.17	1.23
1	D	288	TYR	C-O	-5.47	1.17	1.24
1	C	413	PHE	C-O	-5.45	1.17	1.24
1	D	413	PHE	C-O	-5.44	1.17	1.23
1	E	290	ASN	C-O	-5.43	1.16	1.23
1	D	286	LEU	C-O	-5.42	1.17	1.24
1	C	286	LEU	C-O	-5.40	1.17	1.24
1	B	454	LEU	C-O	-5.24	1.17	1.24
1	E	239	LEU	C-O	-5.06	1.17	1.24
1	C	288	TYR	C-O	-5.05	1.17	1.24

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ASN	CA-C-N	10.52	130.18	119.56
1	A	339	ASN	C-N-CA	10.52	130.18	119.56
1	C	200	ALA	N-CA-C	-10.20	95.06	109.24
1	C	218	ARG	CA-C-N	9.35	131.53	119.84
1	C	218	ARG	C-N-CA	9.35	131.53	119.84
1	C	287	ARG	CA-C-N	-8.62	110.01	122.94
1	C	287	ARG	C-N-CA	-8.62	110.01	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	THR	N-CA-C	8.42	122.44	110.23
1	C	218	ARG	N-CA-C	8.35	120.25	109.64
1	B	379	VAL	N-CA-C	8.16	118.96	110.72
1	B	343	MET	CA-C-N	7.92	127.63	119.56
1	B	343	MET	C-N-CA	7.92	127.63	119.56
1	A	450	LYS	CA-CB-CG	-7.70	98.70	114.10
1	D	239	LEU	N-CA-C	7.43	121.19	112.72
1	D	87[A]	HIS	CA-C-O	7.23	128.79	120.98
1	D	87[B]	HIS	CA-C-O	7.23	128.79	120.98
1	A	100	CYS	N-CA-C	-7.21	103.36	111.07
1	B	103	MET	CB-CG-SD	-7.08	91.46	112.70
1	E	3	VAL	CA-C-N	6.93	126.90	120.03
1	E	3	VAL	C-N-CA	6.93	126.90	120.03
1	A	450	LYS	CB-CG-CD	6.62	126.52	111.30
1	B	339	ASN	CA-C-N	6.53	126.15	119.56
1	B	339	ASN	C-N-CA	6.53	126.15	119.56
1	C	369	CYS	N-CA-C	6.41	120.71	112.12
1	B	342	ALA	CA-C-N	-6.36	117.00	123.10
1	B	342	ALA	C-N-CA	-6.36	117.00	123.10
1	B	87[A]	HIS	CA-C-O	6.04	128.34	121.58
1	B	87[B]	HIS	CA-C-O	6.04	128.34	121.58
1	B	339	ASN	N-CA-C	-6.04	102.14	109.57
1	C	263	PRO	CA-C-N	-5.91	111.90	120.29
1	C	263	PRO	C-N-CA	-5.91	111.90	120.29
1	A	87[A]	HIS	CA-C-O	5.88	127.24	120.60
1	A	87[B]	HIS	CA-C-O	5.88	127.24	120.60
1	B	287	ARG	CA-C-N	-5.71	114.38	122.94
1	B	287	ARG	C-N-CA	-5.71	114.38	122.94
1	D	342	ALA	N-CA-C	5.59	118.34	110.23
1	E	437	THR	O-C-N	5.54	129.09	122.27
1	B	73	GLU	CA-CB-CG	-5.46	103.19	114.10
1	C	368	PHE	N-CA-C	5.41	121.29	114.31
1	D	342	ALA	CA-C-N	-5.34	117.97	123.10
1	D	342	ALA	C-N-CA	-5.34	117.97	123.10
1	A	106	HIS	N-CA-C	5.28	120.00	113.50
1	C	69	MET	N-CA-C	5.25	117.75	111.71
1	C	71	PHE	CA-C-N	-5.25	112.33	120.31
1	C	71	PHE	C-N-CA	-5.25	112.33	120.31
1	B	62	VAL	N-CA-C	5.24	117.93	112.90
1	B	204	GLY	N-CA-C	5.17	118.68	111.19
1	D	288	TYR	N-CA-C	5.10	117.72	109.40
1	E	288	TYR	N-CA-C	5.07	117.23	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	71	PHE	CA-C-N	-5.06	112.61	120.31
1	E	71	PHE	C-N-CA	-5.06	112.61	120.31
1	A	71	PHE	CA-C-N	-5.04	112.66	120.31
1	A	71	PHE	C-N-CA	-5.04	112.66	120.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	LEU	Mainchain
1	E	61	LEU	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	3284	0	3258	70	0
1	B	3262	0	3233	83	0
1	C	3277	0	3252	97	0
1	D	3283	0	3256	63	0
1	E	3267	0	3234	94	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
3	B	1	0	0	0	0
3	D	2	0	0	0	0
All	All	16391	0	16233	379	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 12.

All (379) 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:E:340:PRO:N	1:E:340:PRO:CD	1.70	1.45
1:B:161:GLY:HA3	1:B:167:ILE:CD1	1.54	1.36
1:B:87[B]:HIS:CD2	1:B:132:PHE:HB3	1.63	1.32
1:E:379:VAL:HG13	1:E:410:ASN:ND2	1.65	1.10
1:D:161:GLY:HA3	1:D:167:ILE:HD13	1.34	1.09
1:D:175:THR:HG22	1:E:439:LEU:HD22	1.33	1.07
1:B:161:GLY:HA3	1:B:167:ILE:HD11	1.04	1.03
1:D:161:GLY:HA3	1:D:167:ILE:CD1	1.89	1.03
1:B:161:GLY:CA	1:B:167:ILE:CD1	2.40	0.99
1:C:339:ASN:OD1	1:C:340:PRO:HD2	1.65	0.97
1:E:70:GLY:C	1:E:106:HIS:CE1	2.42	0.97
1:B:87[B]:HIS:HD2	1:B:132:PHE:HB3	0.81	0.97
1:A:439:LEU:HD22	1:E:175:THR:HG21	1.49	0.94
1:B:87[B]:HIS:HD2	1:B:132:PHE:CB	1.78	0.94
1:A:167:ILE:HG12	1:A:433:VAL:HG22	1.47	0.93
1:B:161:GLY:HA3	1:B:167:ILE:HD13	1.48	0.91
1:B:161:GLY:CA	1:B:167:ILE:HD11	1.98	0.91
1:D:139:THR:OG1	1:D:408:ASP:OD1	1.90	0.89
1:E:339:ASN:OD1	1:E:340:PRO:HD2	1.72	0.89
1:B:161:GLY:CA	1:B:167:ILE:HD13	2.04	0.87
1:A:339:ASN:OD1	1:A:340:PRO:HD2	1.74	0.87
1:D:175:THR:CG2	1:E:439:LEU:HD22	2.05	0.86
1:D:63:ARG:HD3	1:E:338:ASP:OD2	1.77	0.85
1:D:103:MET:HE3	1:D:113:THR:OG1	1.79	0.83
1:B:87[B]:HIS:CD2	1:B:132:PHE:CB	2.58	0.83
1:D:175:THR:HG22	1:E:439:LEU:CD2	2.09	0.82
1:D:175:THR:CG2	1:E:439:LEU:CD2	2.58	0.82
1:E:234:THR:HG21	1:E:265:PHE:O	1.79	0.82
1:C:310:LYS:HZ2	1:C:382:GLU:HG3	1.44	0.81
1:E:309:PRO:HG2	1:E:382:GLU:HB3	1.63	0.81
1:E:193:GLN:OE1	1:E:199:THR:HG21	1.61	0.80
1:C:193:GLN:OE1	1:C:199:THR:HG23	1.83	0.79
1:B:74:ASP:OD1	1:B:398:ARG:NH2	2.15	0.78
1:B:289:LYS:NZ	1:B:464:HIS:O	2.15	0.78
1:E:21:LEU:HB3	1:E:265:PHE:CE2	2.20	0.77
1:C:87[A]:HIS:HE1	1:C:133:VAL:CG2	1.98	0.77
1:C:287:ARG:NH1	1:C:430:ASN:HB3	1.99	0.76
1:B:287:ARG:NH2	1:B:430:ASN:HB3	2.00	0.76
1:E:339:ASN:OD1	1:E:340:PRO:CD	2.34	0.76
1:D:194:ILE:CD1	1:D:413:PHE:CE2	2.70	0.75
1:A:161:GLY:HA3	1:A:167:ILE:CD1	2.16	0.75
1:A:346:VAL:O	1:A:352:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ARG:HG3	1:C:63:ARG:HH11	1.52	0.74
1:D:194:ILE:HD11	1:D:413:PHE:CD2	2.22	0.74
1:E:346:VAL:HG11	1:E:351:LEU:HD22	1.68	0.74
1:D:86:PRO:HG2	1:D:303:ALA:HB2	1.69	0.73
1:E:379:VAL:CG1	1:E:410:ASN:ND2	2.50	0.73
1:C:14:ARG:HD2	1:C:264:PHE:CD2	2.24	0.73
1:D:161:GLY:CA	1:D:167:ILE:HD13	2.15	0.73
1:E:190:PRO:HB2	1:E:195:THR:HG23	1.71	0.72
1:B:21:LEU:CB	1:B:265:PHE:CE1	2.73	0.72
1:B:59:PHE:CD2	1:C:335:PHE:CG	2.76	0.72
1:C:287:ARG:NH1	1:C:430:ASN:CG	2.47	0.72
1:E:70:GLY:HA3	1:E:106:HIS:HE1	1.55	0.71
1:D:175:THR:HG21	1:E:439:LEU:HD21	1.73	0.71
1:B:86:PRO:HG2	1:B:303:ALA:HB2	1.71	0.71
1:E:21:LEU:HB3	1:E:265:PHE:CD2	2.25	0.71
1:C:193:GLN:OE1	1:C:199:THR:CG2	2.38	0.71
1:B:23:ALA:HB1	1:B:123:MET:HE1	1.70	0.70
1:C:375:LEU:O	1:C:379:VAL:HG23	1.91	0.70
1:D:339:ASN:OD1	1:D:340:PRO:HD2	1.91	0.70
1:B:287:ARG:HH21	1:B:430:ASN:HB3	1.53	0.70
1:C:287:ARG:NH1	1:C:430:ASN:OD1	2.24	0.70
1:A:14:ARG:HB2	1:A:264:PHE:CE2	2.27	0.69
1:E:21:LEU:CB	1:E:265:PHE:CD2	2.75	0.69
1:B:59:PHE:HB2	1:C:335:PHE:CZ	2.28	0.69
1:E:218:ARG:HB2	1:E:387:ARG:HD3	1.73	0.69
1:A:161:GLY:HA3	1:A:167:ILE:HD13	1.74	0.69
1:C:394:TYR:CE2	1:C:398:ARG:HD2	2.28	0.68
1:C:87[A]:HIS:HE1	1:C:133:VAL:HG22	1.59	0.68
1:C:339:ASN:OD1	1:C:340:PRO:CD	2.39	0.68
1:C:218:ARG:HH21	1:C:219:PRO:HD3	1.59	0.67
1:E:21:LEU:CB	1:E:265:PHE:CE2	2.77	0.67
1:A:177:TRP:CD2	1:A:178:PRO:HD2	2.29	0.67
1:B:21:LEU:HB2	1:B:265:PHE:CE1	2.29	0.67
1:E:167:ILE:HG13	1:E:433:VAL:HG22	1.77	0.67
1:E:346:VAL:O	1:E:352:ARG:NH2	2.28	0.67
1:E:70:GLY:O	1:E:106:HIS:CE1	2.48	0.66
1:A:41:GLN:HB3	1:A:123:MET:HE1	1.79	0.65
1:A:309:PRO:HG2	1:A:382:GLU:HB3	1.79	0.65
1:C:346:VAL:O	1:C:352:ARG:NH2	2.30	0.64
1:A:343:MET:O	1:A:352:ARG:NH1	2.23	0.64
1:C:310:LYS:NZ	1:C:382:GLU:HG3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:MET:HB3	1:D:113:THR:HG23	1.80	0.64
1:B:21:LEU:HB2	1:B:265:PHE:CD1	2.34	0.63
1:B:21:LEU:HB3	1:B:265:PHE:CE1	2.33	0.63
1:D:339:ASN:OD1	1:D:340:PRO:CD	2.47	0.63
1:A:177:TRP:CG	1:A:178:PRO:HD2	2.34	0.63
1:E:2:PHE:HB3	1:E:74:ASP:OD1	1.99	0.63
1:E:346:VAL:HG11	1:E:351:LEU:CD2	2.29	0.63
1:B:318:GLU:OE2	1:B:345:TYR:CE2	2.52	0.62
1:B:74:ASP:OD2	1:B:106:HIS:NE2	2.33	0.62
1:A:57:LEU:HD11	1:A:112:ALA:HB1	1.82	0.61
1:C:167:ILE:HG22	1:C:168:THR:H	1.65	0.61
1:C:287:ARG:NH1	1:C:430:ASN:CB	2.61	0.61
1:A:289:LYS:NZ	1:A:464:HIS:O	2.34	0.61
1:D:177:TRP:CD2	1:D:178:PRO:HD2	2.36	0.61
1:E:70:GLY:CA	1:E:106:HIS:HE1	2.12	0.60
1:B:59:PHE:CZ	1:C:335:PHE:HA	2.37	0.60
1:B:318:GLU:OE2	1:B:345:TYR:HE2	1.85	0.59
1:A:59:PHE:HA	1:A:62:VAL:HG22	1.83	0.59
1:D:194:ILE:CD1	1:D:413:PHE:CD2	2.85	0.59
1:C:87[A]:HIS:CD2	1:C:282:PRO:HG3	2.38	0.59
1:A:228:LEU:HD11	1:A:300:GLU:HB3	1.85	0.58
1:A:465:LEU:HD21	1:E:48:PRO:HB2	1.85	0.58
1:B:21:LEU:CB	1:B:265:PHE:CD1	2.86	0.58
1:C:63:ARG:NE	1:D:338:ASP:OD2	2.36	0.58
1:D:161:GLY:HA3	1:D:167:ILE:HD11	1.82	0.58
1:E:21:LEU:HB2	1:E:265:PHE:CD2	2.38	0.58
1:D:175:THR:HG21	1:E:439:LEU:CD2	2.26	0.58
1:D:77:CYS:SG	1:D:398:ARG:HG2	2.44	0.58
1:E:379:VAL:HG13	1:E:410:ASN:HD22	1.60	0.58
1:C:87[A]:HIS:HE1	1:C:133:VAL:HG23	1.67	0.57
1:A:2:PHE:HB3	1:A:74:ASP:OD1	2.03	0.57
1:E:346:VAL:CG1	1:E:351:LEU:HD22	2.34	0.57
1:B:59:PHE:CD2	1:C:335:PHE:CD1	2.92	0.57
1:D:177:TRP:CG	1:D:178:PRO:HD2	2.39	0.57
1:B:103:MET:HE1	1:B:116:LEU:HD13	1.87	0.57
1:A:74:ASP:OD1	1:A:398:ARG:NH2	2.38	0.57
1:B:343:MET:N	1:B:344:PRO:HD3	2.19	0.57
1:D:194:ILE:HD12	1:D:413:PHE:CE2	2.39	0.57
1:E:23:ALA:HB1	1:E:123:MET:CE	2.34	0.57
1:E:225:LEU:HD12	1:E:305:HIS:HD2	1.70	0.57
1:A:230:ASP:O	1:A:234:THR:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:HB2	1:B:9:THR:OG1	2.06	0.56
1:B:287:ARG:HH21	1:B:430:ASN:CB	2.18	0.56
1:D:175:THR:CG2	1:E:439:LEU:HD21	2.30	0.56
1:E:191:CYS:SG	1:E:195:THR:HG21	2.45	0.56
1:C:77:CYS:SG	1:C:398:ARG:HG2	2.46	0.55
1:C:86:PRO:HG2	1:C:303:ALA:HB2	1.87	0.55
1:B:281:HIS:CG	1:B:282:PRO:HD2	2.41	0.55
1:A:281:HIS:CG	1:A:282:PRO:HD2	2.41	0.55
1:B:59:PHE:CE2	1:C:335:PHE:CB	2.90	0.55
1:C:289:LYS:NZ	1:C:464:HIS:O	2.37	0.55
1:E:86:PRO:HG2	1:E:303:ALA:HB2	1.89	0.55
1:C:69:MET:O	1:C:69:MET:HG3	2.06	0.55
1:D:167:ILE:HG13	1:D:433:VAL:HG22	1.89	0.55
1:E:23:ALA:HB1	1:E:123:MET:HE1	1.89	0.55
1:C:63:ARG:HG3	1:C:63:ARG:NH1	2.20	0.54
1:E:4:PRO:HB2	1:E:81:PHE:CD2	2.43	0.54
1:A:4:PRO:O	1:A:221:LYS:NZ	2.39	0.54
1:C:21:LEU:CB	1:C:265:PHE:CE1	2.90	0.54
1:A:343:MET:C	1:A:352:ARG:HH12	2.14	0.54
1:E:70:GLY:CA	1:E:106:HIS:CE1	2.89	0.54
1:C:167:ILE:HG13	1:C:433:VAL:HG22	1.90	0.54
1:C:63:ARG:HH11	1:C:63:ARG:CG	2.19	0.54
1:C:265:PHE:HE2	1:C:267:PRO:HB3	1.73	0.54
1:C:225:LEU:HD23	1:C:228:LEU:HD23	1.89	0.54
1:D:103:MET:CB	1:D:113:THR:HG23	2.38	0.54
1:C:371:PRO:HB2	1:C:422:VAL:HG22	1.90	0.53
1:E:42:ILE:CD1	1:E:279:LEU:HD13	2.37	0.53
1:C:2:PHE:HB3	1:C:74:ASP:OD1	2.08	0.53
1:A:59:PHE:HE2	1:B:338:ASP:OD2	1.92	0.53
1:A:343:MET:HE2	1:A:346:VAL:HG21	1.90	0.53
1:E:70:GLY:C	1:E:106:HIS:HE1	2.09	0.53
1:A:73:GLU:OE1	1:A:398:ARG:NH1	2.42	0.53
1:E:325:ASN:O	1:E:332:ARG:NH2	2.42	0.53
1:B:59:PHE:CE2	1:C:335:PHE:HA	2.44	0.53
1:E:316:GLN:HB2	1:E:367:LEU:HD22	1.91	0.53
1:A:167:ILE:HG12	1:A:433:VAL:CG2	2.30	0.53
1:B:101:GLU:O	1:B:105:LEU:HD13	2.08	0.53
1:D:48:PRO:HB2	1:E:465:LEU:HD21	1.91	0.53
1:A:218:ARG:O	1:A:387:ARG:NH1	2.43	0.52
1:B:70:GLY:O	1:B:74:ASP:OD2	2.27	0.52
1:E:281:HIS:ND1	1:E:282:PRO:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:O	1:A:62:VAL:HG22	2.09	0.52
1:C:309:PRO:HG2	1:C:382:GLU:HB3	1.90	0.52
1:E:343:MET:HG2	1:E:345:TYR:OH	2.09	0.52
1:C:281:HIS:CG	1:C:282:PRO:HD2	2.45	0.52
1:C:286:LEU:HA	1:C:294:SER:OG	2.10	0.52
1:D:2:PHE:HB3	1:D:74:ASP:OD1	2.10	0.52
1:C:21:LEU:HB2	1:C:265:PHE:CE1	2.45	0.51
1:C:42:ILE:CD1	1:C:279:LEU:HD13	2.39	0.51
1:B:318:GLU:OE2	1:B:345:TYR:OH	2.20	0.51
1:C:41:GLN:NE2	1:C:123:MET:HG3	2.26	0.51
1:C:38:ILE:HD12	1:C:123:MET:HE1	1.93	0.51
1:C:167:ILE:HG22	1:C:168:THR:N	2.25	0.51
1:C:63:ARG:NH1	1:C:63:ARG:CG	2.73	0.51
1:E:225:LEU:HD12	1:E:305:HIS:CD2	2.46	0.51
1:A:352:ARG:O	1:A:356:ARG:HG3	2.11	0.50
1:B:338:ASP:O	1:B:339:ASN:C	2.53	0.50
1:E:108:PRO:O	1:E:114:TYR:OH	2.07	0.50
1:B:168:THR:HG23	1:B:168:THR:O	2.12	0.50
1:A:3:VAL:HG21	1:A:389:PRO:HG3	1.92	0.49
1:B:194:ILE:HD11	1:B:413:PHE:CD2	2.47	0.49
1:E:339:ASN:OD1	1:E:340:PRO:N	2.46	0.49
1:A:21:LEU:HB2	1:A:265:PHE:CD1	2.47	0.49
1:C:14:ARG:HD2	1:C:264:PHE:CE2	2.47	0.49
1:A:167:ILE:CG1	1:A:433:VAL:HG22	2.33	0.49
1:A:306:PRO:HG3	1:A:386:PHE:CG	2.46	0.49
1:B:309:PRO:HG2	1:B:382:GLU:HB3	1.95	0.49
1:C:343:MET:HG2	1:C:345:TYR:OH	2.13	0.49
1:C:218:ARG:NH2	1:C:219:PRO:HD3	2.25	0.49
1:E:440:ASP:OD1	1:E:443:ARG:NH1	2.46	0.49
1:D:218:ARG:HD3	1:D:388:LEU:O	2.13	0.49
1:B:306:PRO:HG3	1:B:386:PHE:CD1	2.48	0.49
1:E:70:GLY:O	1:E:106:HIS:NE2	2.45	0.49
1:D:6:GLN:HB2	1:D:9:THR:OG1	2.13	0.48
1:A:21:LEU:HB2	1:A:265:PHE:CE1	2.48	0.48
1:E:449:LEU:HD13	1:E:456:LEU:HD12	1.95	0.48
1:E:397:LEU:HD11	1:E:406:LEU:HD22	1.95	0.48
1:B:59:PHE:CE2	1:C:335:PHE:HB3	2.47	0.48
1:E:196:ASP:OD2	1:E:199:THR:HG23	2.14	0.48
1:D:57:LEU:O	1:D:61:LEU:HG	2.14	0.48
1:D:328:LYS:HG3	1:D:330:VAL:HG22	1.95	0.48
1:B:194:ILE:O	1:B:453:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ILE:CD1	1:C:123:MET:HE1	2.44	0.48
1:D:61:LEU:HD11	1:D:103:MET:HE1	1.94	0.48
1:A:316:GLN:HB2	1:A:367:LEU:HD22	1.96	0.47
1:A:281:HIS:CD2	1:A:282:PRO:HD2	2.49	0.47
1:A:306:PRO:HG3	1:A:386:PHE:CD1	2.49	0.47
1:B:103:MET:HB2	1:B:103:MET:HE3	1.70	0.47
1:C:167:ILE:CG1	1:C:433:VAL:HG22	2.44	0.47
1:E:59:PHE:HA	1:E:62:VAL:HG22	1.95	0.47
1:C:88:CYS:HB2	1:C:300:GLU:OE2	2.15	0.47
1:B:310:LYS:NZ	1:B:382:GLU:HG3	2.30	0.47
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.72	0.47
1:A:87[A]:HIS:HE1	1:A:133:VAL:CG2	2.28	0.47
1:C:225:LEU:HD12	1:C:305:HIS:HD2	1.79	0.47
1:A:343:MET:HG2	1:A:345:TYR:OH	2.14	0.47
1:E:25:LEU:HD11	1:E:265:PHE:HZ	1.80	0.47
1:E:146:LEU:HA	1:E:146:LEU:HD23	1.72	0.47
1:A:41:GLN:NE2	1:A:123:MET:HE2	2.30	0.47
1:B:375:LEU:O	1:B:379:VAL:HG23	2.15	0.47
1:B:218:ARG:HB2	1:B:387:ARG:HD2	1.97	0.47
1:E:167:ILE:CG1	1:E:433:VAL:HG22	2.44	0.47
1:E:214:CYS:O	1:E:390:ARG:NH2	2.47	0.47
1:C:408:ASP:OD1	1:C:408:ASP:N	2.48	0.46
1:C:21:LEU:HB3	1:C:265:PHE:CE1	2.51	0.46
1:C:87[A]:HIS:CE1	1:C:133:VAL:CG2	2.90	0.46
1:A:325:ASN:O	1:A:332:ARG:NH2	2.48	0.46
1:A:379:VAL:HG13	1:A:410:ASN:ND2	2.30	0.46
1:D:455:ASP:O	1:D:456:LEU:HD23	2.16	0.46
1:A:281:HIS:CE1	1:A:282:PRO:HD2	2.50	0.46
1:C:14:ARG:NH1	1:C:264:PHE:HA	2.31	0.46
1:C:175:THR:HG22	1:D:458:HIS:HE1	1.80	0.46
1:C:89:TRP:HD1	1:C:280:MET:HB2	1.81	0.46
1:C:119:PRO:HA	1:C:123:MET:CE	2.46	0.46
1:C:218:ARG:N	1:C:218:ARG:HD2	2.25	0.46
1:E:229:ILE:O	1:E:233:SER:OG	2.29	0.46
1:B:175:THR:HG21	1:C:460:SER:HB3	1.98	0.46
1:D:86:PRO:CG	1:D:303:ALA:HB2	2.44	0.46
1:E:17:LEU:HD23	1:E:17:LEU:HA	1.74	0.46
1:C:21:LEU:HB2	1:C:265:PHE:CD1	2.51	0.45
1:A:228:LEU:CD1	1:A:300:GLU:HB3	2.46	0.45
1:C:6:GLN:HG2	1:C:221:LYS:HD2	1.97	0.45
1:A:129:LEU:HA	1:A:133:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:HIS:CD2	1:B:100:CYS:HB3	2.51	0.45
1:D:449:LEU:HD23	1:D:449:LEU:HA	1.75	0.45
1:E:228:LEU:HD12	1:E:232:TRP:CD1	2.52	0.45
1:A:325:ASN:HB2	1:A:327:VAL:HG23	1.97	0.45
1:C:347:SER:OG	1:C:348:ASP:N	2.50	0.45
1:D:130:HIS:CE1	1:D:136:CYS:HB2	2.51	0.45
1:E:138:LYS:NZ	1:E:414:ASP:OD2	2.43	0.45
1:B:42:ILE:CD1	1:B:279:LEU:HD13	2.47	0.45
1:E:3:VAL:HA	1:E:4:PRO:HD3	1.75	0.45
1:E:61:LEU:HD11	1:E:103:MET:HE1	1.97	0.45
1:A:135:LYS:HD3	1:A:138:LYS:HD2	1.97	0.45
1:A:448:GLN:OE1	1:A:451:ARG:NH1	2.48	0.45
1:B:77:CYS:SG	1:B:398:ARG:HG2	2.57	0.45
1:B:87[A]:HIS:CD2	1:B:423:PHE:HZ	2.35	0.45
1:B:340:PRO:HA	1:B:356:ARG:HH22	1.82	0.45
1:C:87[A]:HIS:CE1	1:C:133:VAL:HG23	2.49	0.45
1:D:25:LEU:HD23	1:D:276:GLY:C	2.41	0.45
1:B:59:PHE:CE2	1:C:335:PHE:CG	3.05	0.45
1:D:323:ILE:HG23	1:D:325:ASN:OD1	2.17	0.45
1:E:265:PHE:HE1	1:E:267:PRO:HB3	1.81	0.45
1:E:318:GLU:OE2	1:E:345:TYR:HE2	2.00	0.45
1:C:325:ASN:HB2	1:C:327:VAL:HG23	1.99	0.44
1:D:288:TYR:CE2	1:D:293:ALA:HB2	2.52	0.44
1:A:103:MET:HE1	1:A:116:LEU:HD13	2.00	0.44
1:C:426:LYS:HA	1:C:426:LYS:HD2	1.83	0.44
1:B:394:TYR:O	1:B:398:ARG:HG3	2.18	0.44
1:D:167:ILE:CG1	1:D:433:VAL:HG22	2.47	0.44
1:D:379:VAL:HG13	1:D:410:ASN:ND2	2.32	0.44
1:E:318:GLU:OE2	1:E:345:TYR:CE2	2.70	0.44
1:A:21:LEU:CB	1:A:265:PHE:CE1	3.00	0.44
1:B:225:LEU:HD23	1:B:225:LEU:HA	1.69	0.44
1:C:190:PRO:HB3	1:C:195:THR:O	2.18	0.44
1:E:25:LEU:HD11	1:E:265:PHE:CZ	2.52	0.44
1:C:218:ARG:HD2	1:C:218:ARG:HA	1.53	0.44
1:E:52:CYS:HB3	1:E:55:CYS:HB2	2.00	0.44
1:C:312:LEU:HA	1:C:312:LEU:HD23	1.81	0.44
1:D:103:MET:HB3	1:D:113:THR:CG2	2.47	0.44
1:D:305:HIS:HA	1:D:306:PRO:HD3	1.87	0.44
1:A:3:VAL:HG22	1:A:394:TYR:CZ	2.53	0.44
1:A:72:PHE:N	1:A:72:PHE:CD1	2.83	0.44
1:B:21:LEU:HB3	1:B:265:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:MET:HE1	1:A:116:LEU:CD1	2.48	0.43
1:B:107:PHE:O	1:B:113:THR:OG1	2.23	0.43
1:B:343:MET:CE	1:B:356:ARG:HG3	2.48	0.43
1:E:22:ALA:N	1:E:265:PHE:HE2	2.16	0.43
1:E:145:ILE:HD13	1:E:145:ILE:HA	1.80	0.43
1:D:17:LEU:HD11	1:D:97:ALA:HB2	1.99	0.43
1:E:311:ALA:HB2	1:E:346:VAL:HG22	2.00	0.43
1:A:87[A]:HIS:HE1	1:A:133:VAL:HG23	1.82	0.43
1:B:287:ARG:HH21	1:B:430:ASN:CG	2.27	0.43
1:A:359:THR:OG1	1:A:362:GLU:HG3	2.19	0.43
1:B:2:PHE:HB3	1:B:74:ASP:OD1	2.18	0.43
1:D:101:GLU:O	1:D:105:LEU:HD13	2.18	0.43
1:D:327:VAL:HG12	1:D:332:ARG:HG3	2.00	0.43
1:C:130:HIS:CE1	1:C:136:CYS:HB2	2.53	0.43
1:D:343:MET:HG2	1:D:345:TYR:OH	2.18	0.43
1:A:196:ASP:OD1	1:A:198:THR:HB	2.18	0.43
1:B:306:PRO:HG3	1:B:386:PHE:CG	2.54	0.43
1:D:63:ARG:HD3	1:E:338:ASP:CG	2.41	0.43
1:B:161:GLY:HA2	1:B:167:ILE:HD13	1.93	0.43
1:D:13:HIS:HE1	1:D:101:GLU:OE1	2.01	0.43
1:D:207:GLU:OE2	1:D:210:ARG:NH2	2.46	0.43
1:C:59:PHE:HE2	1:D:338:ASP:OD2	2.02	0.42
1:D:4:PRO:O	1:D:221:LYS:NZ	2.51	0.42
1:B:59:PHE:CE2	1:C:335:PHE:CA	3.02	0.42
1:C:87[A]:HIS:CE1	1:C:133:VAL:HG22	2.45	0.42
1:C:218:ARG:NH2	1:C:219:PRO:CD	2.83	0.42
1:C:449:LEU:HA	1:C:449:LEU:HD23	1.76	0.42
1:E:396:LYS:NZ	1:E:400:SER:HB2	2.34	0.42
1:A:77:CYS:SG	1:A:398:ARG:HG2	2.60	0.42
1:C:119:PRO:HA	1:C:123:MET:HE3	2.01	0.42
1:C:439:LEU:HD23	1:C:442:ILE:HD12	2.01	0.42
1:A:375:LEU:O	1:A:379:VAL:HG23	2.20	0.42
1:B:70:GLY:C	1:B:106:HIS:CE1	2.97	0.42
1:B:354:LEU:C	1:B:354:LEU:HD23	2.44	0.42
1:B:365:LYS:HA	1:B:369:CYS:HB2	2.01	0.42
1:C:17:LEU:HD11	1:C:97:ALA:HB2	2.01	0.42
1:C:343:MET:HA	1:C:345:TYR:CE1	2.55	0.42
1:A:296:CYS:O	1:A:300:GLU:HG2	2.20	0.42
1:C:21:LEU:CB	1:C:265:PHE:CD1	3.02	0.42
1:C:103:MET:HB3	1:C:113:THR:HG23	2.00	0.42
1:E:192:CYS:H	1:E:195:THR:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:LYS:HA	1:D:426:LYS:HD2	1.79	0.42
1:C:218:ARG:HA	1:C:219:PRO:HD3	1.37	0.42
1:E:135:LYS:HD3	1:E:138:LYS:HD2	2.02	0.42
1:E:397:LEU:CD1	1:E:406:LEU:HD22	2.50	0.42
1:A:16:GLU:OE2	1:A:115:GLY:N	2.53	0.42
1:A:88:CYS:HB2	1:A:300:GLU:OE2	2.19	0.42
1:B:336:VAL:HG12	1:B:337:LEU:HD23	2.02	0.42
1:E:225:LEU:HA	1:E:225:LEU:HD23	1.87	0.42
1:A:42:ILE:CD1	1:A:279:LEU:HD13	2.49	0.41
1:C:161:GLY:HA3	1:C:167:ILE:HD13	2.02	0.41
1:B:116:LEU:HD23	1:B:117:PHE:CZ	2.55	0.41
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.81	0.41
1:E:449:LEU:HD23	1:E:449:LEU:HA	1.87	0.41
1:C:63:ARG:CD	1:D:338:ASP:OD2	2.69	0.41
1:E:281:HIS:CG	1:E:282:PRO:HD2	2.55	0.41
1:B:371:PRO:HB2	1:B:422:VAL:HG22	2.02	0.41
1:C:193:GLN:OE1	1:C:199:THR:HG21	2.18	0.41
1:D:233:SER:HB3	1:D:239:LEU:HD12	2.01	0.41
1:A:86:PRO:HG2	1:A:303:ALA:HB2	2.02	0.41
1:A:426:LYS:HA	1:A:426:LYS:HD2	1.91	0.41
1:B:265:PHE:HE2	1:B:267:PRO:HB3	1.85	0.41
1:E:220:THR:HG22	1:E:387:ARG:HH12	1.85	0.41
1:E:281:HIS:CD2	1:E:295:VAL:HG13	2.55	0.41
1:B:426:LYS:HA	1:B:426:LYS:HD2	1.85	0.41
1:C:146:LEU:HA	1:C:146:LEU:HD23	1.71	0.41
1:E:3:VAL:O	1:E:6:GLN:HG3	2.20	0.41
1:E:161:GLY:HA3	1:E:167:ILE:HD13	2.02	0.41
1:B:61:LEU:HB3	1:B:107:PHE:CE2	2.56	0.41
1:C:218:ARG:HH21	1:C:218:ARG:HA	1.86	0.41
1:E:71:PHE:N	1:E:106:HIS:CE1	2.88	0.41
1:A:408:ASP:OD1	1:A:408:ASP:N	2.54	0.41
1:B:150:ASN:O	1:B:153:PHE:HB3	2.21	0.41
1:B:319:VAL:O	1:B:332:ARG:HD3	2.20	0.41
1:B:382:GLU:H	1:B:382:GLU:CD	2.25	0.41
1:C:161:GLY:HA3	1:C:167:ILE:CD1	2.51	0.41
1:D:325:ASN:O	1:D:332:ARG:NH2	2.53	0.41
1:E:192:CYS:H	1:E:195:THR:HG22	1.86	0.41
1:D:125:ILE:HD12	1:D:125:ILE:HA	1.86	0.40
1:E:265:PHE:CE1	1:E:267:PRO:HB3	2.55	0.40
1:A:48:PRO:HB2	1:B:465:LEU:HD21	2.03	0.40
1:A:123:MET:HE3	1:A:123:MET:HB2	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LYS:NZ	1:C:414:ASP:OD2	2.40	0.40
1:E:396:LYS:HZ3	1:E:400:SER:HB2	1.86	0.40
1:A:52:CYS:HB3	1:A:55:CYS:HB2	2.04	0.40
1:B:47:GLN:HA	1:B:48:PRO:HD3	1.94	0.40
1:E:21:LEU:C	1:E:265:PHE:HE2	2.29	0.40
1:A:130:HIS:CE1	1:A:136:CYS:HB2	2.57	0.40
1:B:318:GLU:OE2	1:B:345:TYR:CZ	2.74	0.40
1:C:297:LEU:HD12	1:C:297:LEU:HA	1.95	0.40
1:D:337:LEU:HD22	1:D:356:ARG:HG2	2.03	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	416/467 (89%)	409 (98%)	7 (2%)	0	100	100
1	B	415/467 (89%)	407 (98%)	8 (2%)	0	100	100
1	C	415/467 (89%)	403 (97%)	12 (3%)	0	100	100
1	D	417/467 (89%)	411 (99%)	6 (1%)	0	100	100
1	E	415/467 (89%)	408 (98%)	7 (2%)	0	100	100
All	All	2078/2335 (89%)	2038 (98%)	40 (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	361/407 (89%)	359 (99%)	2 (1%)	78	88
1	B	356/407 (88%)	355 (100%)	1 (0%)	86	93
1	C	359/407 (88%)	358 (100%)	1 (0%)	86	93
1	D	360/407 (88%)	359 (100%)	1 (0%)	86	93
1	E	358/407 (88%)	358 (100%)	0	100	100
All	All	1794/2035 (88%)	1789 (100%)	5 (0%)	86	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ILE
1	A	339	ASN
1	B	62	VAL
1	C	218	ARG
1	D	207	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	B	43	HIS
1	B	47	GLN
1	B	313	GLN
1	B	316	GLN
1	B	430	ASN
1	C	313	GLN
1	C	316	GLN
1	D	313	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	425/467 (91%)	0.64	39 (9%)	14 12	22, 55, 87, 141	1 (0%)
1	B	424/467 (90%)	0.68	40 (9%)	14 11	32, 58, 95, 144	1 (0%)
1	C	424/467 (90%)	0.74	49 (11%)	9 7	20, 59, 97, 155	1 (0%)
1	D	426/467 (91%)	0.77	50 (11%)	9 7	24, 58, 92, 163	1 (0%)
1	E	425/467 (91%)	1.08	77 (18%)	3 2	42, 65, 108, 165	0
All	All	2124/2335 (90%)	0.78	255 (12%)	9 7	20, 59, 98, 165	4 (0%)

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	269	LEU	7.4
1	A	265	PHE	6.0
1	D	240	ASP	5.7
1	D	113	THR	5.5
1	C	263	PRO	5.4
1	D	69	MET	5.4
1	D	68	PRO	5.0
1	C	168	THR	4.9
1	B	265	PHE	4.9
1	D	112	ALA	4.8
1	E	168	THR	4.8
1	E	131	PHE	4.7
1	C	202	ALA	4.7
1	E	270	GLN	4.6
1	B	269	LEU	4.6
1	D	168	THR	4.5
1	B	215	GLY	4.5
1	B	168	THR	4.4
1	A	178	PRO	4.3
1	A	69	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	270	GLN	4.3
1	E	202	ALA	4.2
1	D	178	PRO	4.2
1	C	270	GLN	4.2
1	E	263	PRO	4.2
1	B	112	ALA	4.2
1	C	68	PRO	4.1
1	D	189	THR	4.1
1	E	441	ILE	4.1
1	E	68	PRO	4.0
1	D	263	PRO	4.0
1	A	173	PHE	3.9
1	D	335	PHE	3.8
1	C	200	ALA	3.8
1	B	59	PHE	3.8
1	C	265	PHE	3.8
1	E	343	MET	3.8
1	E	201	PRO	3.8
1	C	201	PRO	3.7
1	E	73	GLU	3.7
1	D	408	ASP	3.7
1	E	112	ALA	3.7
1	E	341	PHE	3.7
1	E	69	MET	3.7
1	D	271	ALA	3.7
1	A	266	SER	3.6
1	E	435	LYS	3.6
1	B	263	PRO	3.6
1	D	28	GLU	3.6
1	C	437	THR	3.6
1	B	271	ALA	3.6
1	C	391	GLU	3.6
1	D	59	PHE	3.5
1	E	434	GLY	3.5
1	B	266	SER	3.5
1	B	31	GLU	3.5
1	E	305	HIS	3.4
1	D	215	GLY	3.4
1	E	265	PHE	3.4
1	E	87	HIS	3.4
1	E	207	GLU	3.4
1	C	208	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	379	VAL	3.4
1	B	69	MET	3.4
1	B	173	PHE	3.4
1	E	189	THR	3.4
1	E	176	SER	3.4
1	C	38	ILE	3.3
1	B	25	LEU	3.3
1	E	71	PHE	3.3
1	A	68	PRO	3.2
1	A	175	THR	3.2
1	D	228	LEU	3.2
1	A	198	THR	3.2
1	C	39	MET	3.2
1	A	107	PHE	3.1
1	E	266	SER	3.1
1	C	2	PHE	3.1
1	E	335	PHE	3.1
1	D	216	ALA	3.1
1	B	240	ASP	3.1
1	C	403	ALA	3.1
1	A	392	GLN	3.0
1	D	72	PHE	3.0
1	B	216	ALA	3.0
1	C	324	GLU	3.0
1	E	200	ALA	3.0
1	E	394	TYR	3.0
1	B	341	PHE	3.0
1	A	202	ALA	3.0
1	E	240	ASP	3.0
1	D	114	TYR	2.9
1	E	143	GLU	2.9
1	E	389	PRO	2.9
1	A	464	HIS	2.9
1	C	317	CYS	2.9
1	A	263	PRO	2.9
1	B	107	PHE	2.9
1	A	112	ALA	2.9
1	E	386	PHE	2.9
1	D	175	THR	2.9
1	E	15	ASP	2.9
1	C	271	ALA	2.8
1	B	87[A]	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	351	LEU	2.8
1	D	239	LEU	2.8
1	D	313	GLN	2.8
1	A	3	VAL	2.8
1	D	391	GLU	2.8
1	B	26	LEU	2.8
1	B	62	VAL	2.8
1	B	323	ILE	2.7
1	E	229	ILE	2.7
1	E	405	GLN	2.7
1	E	177	TRP	2.7
1	E	388	LEU	2.7
1	E	216	ALA	2.7
1	E	2	PHE	2.7
1	D	270	GLN	2.7
1	C	215	GLY	2.7
1	A	100	CYS	2.7
1	D	388	LEU	2.7
1	C	217	SER	2.7
1	A	297	LEU	2.7
1	B	335	PHE	2.7
1	A	109	GLU	2.7
1	C	203	SER	2.7
1	B	39	MET	2.7
1	C	112	ALA	2.6
1	D	225	LEU	2.6
1	E	324	GLU	2.6
1	D	63	ARG	2.6
1	C	404	GLY	2.6
1	E	197	THR	2.6
1	E	208	LEU	2.6
1	C	173	PHE	2.6
1	E	423	PHE	2.6
1	B	450	LYS	2.6
1	D	144	LYS	2.6
1	E	351	LEU	2.5
1	C	443	ARG	2.5
1	D	440	ASP	2.5
1	E	322	HIS	2.5
1	E	453	ARG	2.5
1	B	15	ASP	2.5
1	B	440	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	15	ASP	2.5
1	E	119	PRO	2.5
1	C	220	THR	2.5
1	D	107	PHE	2.5
1	C	343	MET	2.5
1	A	338	ASP	2.5
1	E	193	GLN	2.5
1	E	215	GLY	2.5
1	E	392	GLN	2.5
1	E	198	THR	2.4
1	C	34	LEU	2.4
1	A	240	ASP	2.4
1	A	201	PRO	2.4
1	E	70	GLY	2.4
1	E	395	LYS	2.4
1	B	322	HIS	2.4
1	E	6	GLN	2.4
1	C	216	ALA	2.4
1	E	173	PHE	2.4
1	C	73	GLU	2.4
1	E	339	ASN	2.4
1	E	86	PRO	2.4
1	C	310	LYS	2.4
1	B	167	ILE	2.4
1	D	317	CYS	2.4
1	B	406	LEU	2.4
1	E	338	ASP	2.3
1	B	119	PRO	2.3
1	C	69	MET	2.3
1	A	38	ILE	2.3
1	D	103	MET	2.3
1	E	203	SER	2.3
1	E	387	ARG	2.3
1	A	117	PHE	2.3
1	C	335	PHE	2.3
1	C	341	PHE	2.3
1	C	379	VAL	2.3
1	D	297	LEU	2.3
1	E	317	CYS	2.3
1	A	39	MET	2.3
1	B	467	ALA	2.3
1	E	313	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	269	LEU	2.3
1	C	36	ASN	2.3
1	E	39	MET	2.3
1	A	437	THR	2.3
1	A	104	HIS	2.3
1	C	143	GLU	2.3
1	D	111	GLU	2.3
1	D	19	LYS	2.3
1	A	59	PHE	2.2
1	C	107	PHE	2.2
1	A	119	PRO	2.2
1	A	267	PRO	2.2
1	A	207	GLU	2.2
1	A	399	ALA	2.2
1	B	29	HIS	2.2
1	B	111	GLU	2.2
1	A	177	TRP	2.2
1	E	223	SER	2.2
1	D	62	VAL	2.2
1	E	439	LEU	2.2
1	D	423	PHE	2.2
1	E	72	PHE	2.2
1	A	317	CYS	2.2
1	C	119	PRO	2.2
1	D	119	PRO	2.2
1	E	190	PRO	2.2
1	C	175	THR	2.2
1	E	175	THR	2.2
1	D	173	PHE	2.2
1	B	68	PRO	2.2
1	E	219	PRO	2.2
1	E	77	CYS	2.2
1	D	29	HIS	2.2
1	E	437	THR	2.2
1	D	454	LEU	2.2
1	E	107	PHE	2.2
1	B	434	GLY	2.2
1	E	403	ALA	2.2
1	C	269	LEU	2.1
1	D	323	ILE	2.1
1	D	115	GLY	2.1
1	B	63	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	34	LEU	2.1
1	B	396	LYS	2.1
1	D	116	LEU	2.1
1	C	29	HIS	2.1
1	D	90	THR	2.1
1	B	310	LYS	2.1
1	E	396	LYS	2.1
1	B	28	GLU	2.1
1	E	127	LEU	2.1
1	D	87[A]	HIS	2.1
1	A	73	GLU	2.1
1	E	5	TRP	2.1
1	D	143	GLU	2.0
1	A	264	PHE	2.0
1	A	341	PHE	2.0
1	D	2	PHE	2.0
1	A	450	LYS	2.0
1	C	109	GLU	2.0
1	C	401	ALA	2.0
1	C	322	HIS	2.0
1	A	15	ASP	2.0
1	C	37	PRO	2.0
1	D	38	ILE	2.0
1	E	306	PRO	2.0
1	C	174	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	501	1/1	0.98	0.06	49,49,49,49	0
2	ZN	A	502	1/1	0.98	0.06	42,42,42,42	0
2	ZN	E	501	1/1	0.98	0.05	50,50,50,50	0
2	ZN	E	503	1/1	0.98	0.07	54,54,54,54	0
2	ZN	B	502	1/1	0.99	0.06	46,46,46,46	0
2	ZN	C	502	1/1	0.99	0.05	46,46,46,46	0
2	ZN	D	501	1/1	0.99	0.07	50,50,50,50	0
2	ZN	D	502	1/1	0.99	0.05	47,47,47,47	0
2	ZN	D	503	1/1	0.99	0.04	50,50,50,50	0
2	ZN	A	503	1/1	0.99	0.06	45,45,45,45	0
2	ZN	E	502	1/1	0.99	0.03	51,51,51,51	0
2	ZN	B	501	1/1	0.99	0.05	48,48,48,48	0
2	ZN	C	501	1/1	1.00	0.04	46,46,46,46	0
2	ZN	B	503	1/1	1.00	0.06	47,47,47,47	0
2	ZN	C	503	1/1	1.00	0.07	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.