



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:02 PM UTC

PDB ID : 5CUV / pdb_00005cuv
Title : Crystal structure of Trypanosoma cruzi Vacuolar Soluble Pyrophosphatases in apo form
Authors : Ko, T.P.; Yang, Y.Y.; Liu, W.D.; Zheng, Y.Y.; Chen, C.C.; Guo, R.T.
Deposited on : 2015-07-25
Resolution : 2.62 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

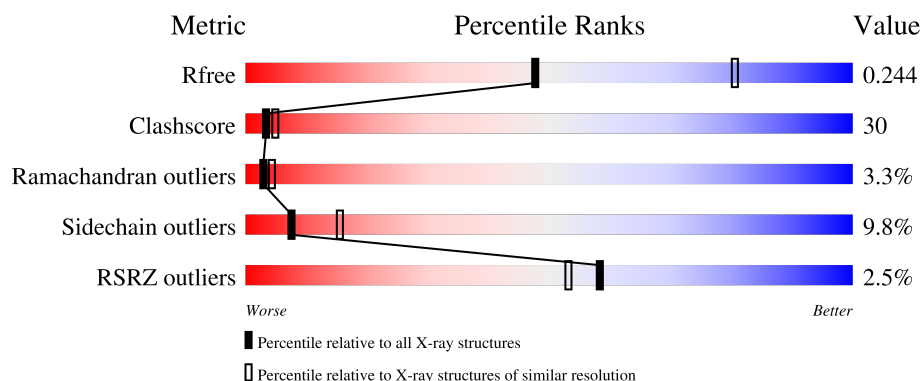
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	414	47% 35% 10% 8% 47% 35% 10% 8%
1	B	414	46% 34% 9% 8% 46% 34% 9% 8%

2 Entry composition [i](#)

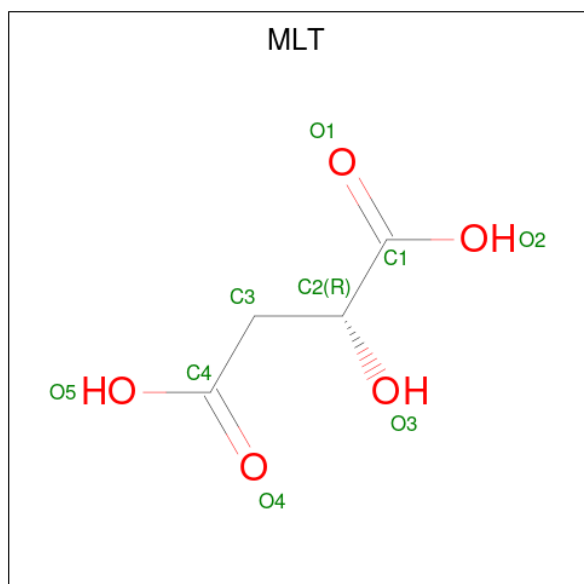
There are 4 unique types of molecules in this entry. The entry contains 6578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acidocalcisomal pyrophosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	Se	0	0	0
			3125	2015	519	567	8	16			
1	B	379	Total	C	N	O	S	Se	0	0	0
			3096	1997	515	560	8	16			

- Molecule 2 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0

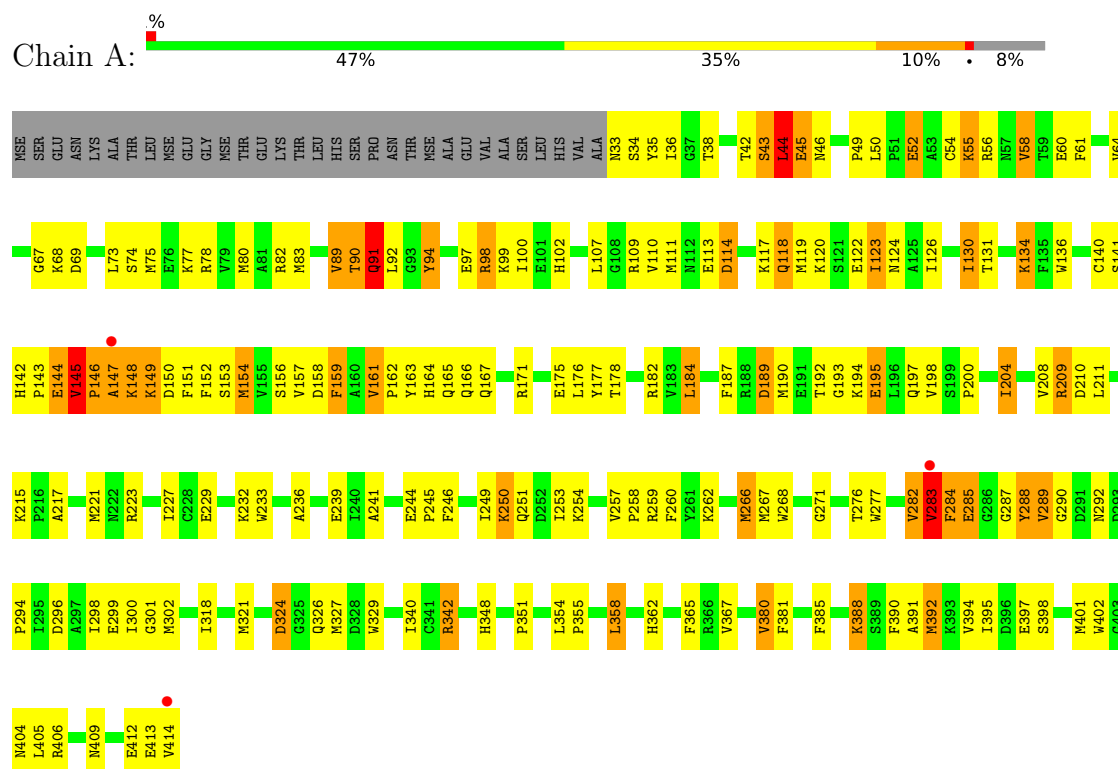
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total 180	O 180	0	0
4	B	166	Total 166	O 166	0	0

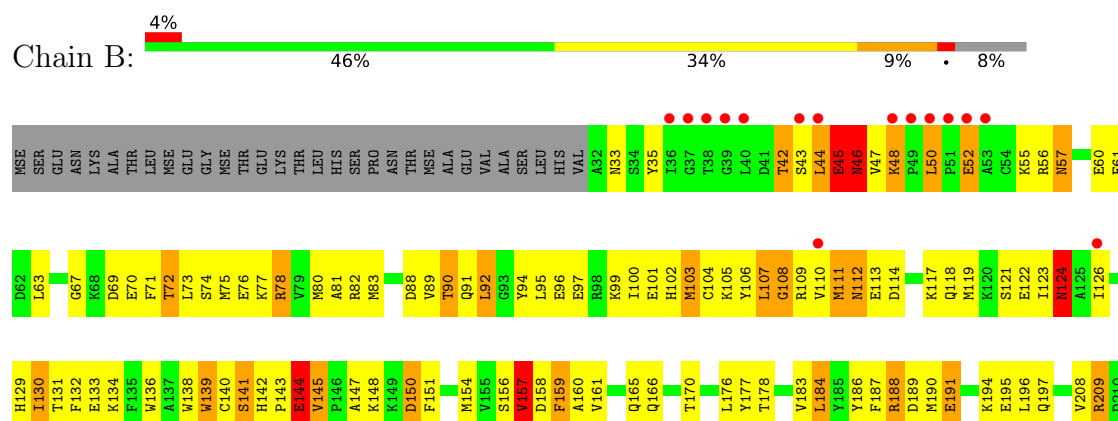
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acidocalcisomal pyrophosphatase



• Molecule 1: Acidocalcisomal pyrophosphatase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.52Å 103.02Å 157.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.62 25.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.4 (25.00-2.62) 97.2 (25.00-2.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.11 (at 2.60Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.177 , 0.235 0.189 , 0.244	Depositor DCC
R_{free} test set	1167 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6578	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.96% 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

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

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	1.37	31/3196 (1.0%)	1.41	38/4294 (0.9%)
1	B	1.30	26/3167 (0.8%)	1.39	44/4256 (1.0%)
All	All	1.33	57/6363 (0.9%)	1.40	82/8550 (1.0%)

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 (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	327	MSE	C-O	-16.26	1.04	1.24
1	A	302	MSE	C-O	-15.88	1.03	1.24
1	A	154	MSE	C-O	-15.71	1.02	1.24
1	A	266	MSE	C-O	-15.62	1.04	1.23
1	B	221	MSE	C-O	-15.04	1.05	1.24
1	B	321	MSE	C-O	-12.19	1.09	1.23
1	A	154	MSE	N-CA	-11.88	1.31	1.46
1	A	154	MSE	CA-C	-11.64	1.37	1.52
1	B	302	MSE	C-O	-11.07	1.09	1.24
1	B	221	MSE	CA-C	-10.63	1.38	1.52
1	B	327	MSE	CA-C	-10.35	1.39	1.52
1	A	267	MSE	C-O	-9.51	1.10	1.24
1	A	119	MSE	C-O	-9.29	1.13	1.24
1	A	266	MSE	N-CA	-8.82	1.34	1.46
1	A	392	MSE	C-O	-8.81	1.13	1.24
1	B	103	MSE	C-O	-8.80	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	MSE	CA-C	-8.71	1.41	1.52
1	B	350	VAL	CA-CB	8.64	1.58	1.54
1	B	103	MSE	C-N	-8.62	1.22	1.33
1	A	266	MSE	CA-C	-8.24	1.42	1.52
1	A	392	MSE	N-CA	-8.07	1.36	1.46
1	B	302	MSE	CA-C	-8.00	1.41	1.52
1	A	267	MSE	N-CA	-7.87	1.35	1.46
1	B	327	MSE	SE-CE	-7.62	1.72	1.95
1	B	327	MSE	N-CA	-7.62	1.36	1.46
1	A	392	MSE	SE-CE	-7.51	1.73	1.95
1	A	154	MSE	SE-CE	-7.48	1.73	1.95
1	A	302	MSE	C-N	-7.37	1.22	1.33
1	B	302	MSE	C-N	-7.31	1.23	1.33
1	B	302	MSE	N-CA	-7.09	1.36	1.46
1	A	283	VAL	CA-CB	7.00	1.63	1.54
1	A	267	MSE	CA-CB	-6.86	1.42	1.53
1	B	321	MSE	CA-C	-6.63	1.45	1.52
1	A	154	MSE	C-N	-6.54	1.25	1.33
1	A	302	MSE	CA-C	-6.52	1.43	1.52
1	B	184	LEU	CA-C	6.45	1.61	1.52
1	A	154	MSE	CG-SE	-6.37	1.76	1.95
1	B	221	MSE	N-CA	-6.33	1.38	1.46
1	B	321	MSE	SE-CE	-6.13	1.77	1.95
1	A	111	MSE	CA-C	-6.12	1.45	1.53
1	B	230	ILE	CA-C	-6.11	1.46	1.52
1	A	111	MSE	C-O	-6.00	1.15	1.23
1	B	221	MSE	C-N	-5.81	1.26	1.33
1	B	111	MSE	CA-C	-5.79	1.45	1.52
1	B	103	MSE	N-CA	-5.77	1.39	1.46
1	A	119	MSE	C-N	-5.68	1.26	1.33
1	B	300	ILE	CA-CB	5.60	1.60	1.54
1	B	221	MSE	CA-CB	-5.54	1.45	1.53
1	A	380	VAL	CA-CB	-5.42	1.47	1.54
1	B	302	MSE	SE-CE	-5.35	1.79	1.95
1	A	302	MSE	SE-CE	-5.34	1.79	1.95
1	A	154	MSE	CA-CB	-5.31	1.45	1.53
1	A	266	MSE	SE-CE	-5.31	1.79	1.95
1	B	111	MSE	N-CA	-5.18	1.39	1.46
1	A	204	ILE	CA-C	5.13	1.58	1.52
1	A	119	MSE	CA-C	-5.12	1.46	1.52
1	A	358	LEU	CA-C	5.02	1.59	1.52

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	MSE	CG-SE-CE	-15.53	64.77	98.92
1	B	321	MSE	CB-CA-C	-10.94	89.36	109.37
1	B	321	MSE	CG-SE-CE	9.83	120.55	98.92
1	B	300	ILE	N-CA-C	9.74	120.58	111.91
1	B	367	VAL	N-CA-C	9.16	120.85	112.43
1	A	267	MSE	CG-SE-CE	-8.83	79.50	98.92
1	B	103	MSE	CG-SE-CE	8.76	118.20	98.92
1	A	367	VAL	N-CA-C	8.63	120.37	112.43
1	A	282	VAL	N-CA-C	-8.57	98.52	109.58
1	A	204	ILE	CA-C-N	-8.51	110.99	119.76
1	A	204	ILE	C-N-CA	-8.51	110.99	119.76
1	A	209	ARG	N-CA-C	8.51	122.77	109.07
1	A	285	GLU	N-CA-C	8.49	123.38	112.34
1	B	157	VAL	CA-C-N	-8.38	110.36	122.94
1	B	157	VAL	C-N-CA	-8.38	110.36	122.94
1	A	189	ASP	N-CA-C	-8.31	97.18	109.15
1	A	161	VAL	CA-C-N	8.28	128.43	120.31
1	A	161	VAL	C-N-CA	8.28	128.43	120.31
1	B	103	MSE	CA-C-O	8.21	129.44	120.82
1	A	388	LYS	N-CA-C	7.99	119.98	111.28
1	A	159	PHE	N-CA-C	-7.81	97.91	109.62
1	B	103	MSE	O-C-N	-7.50	114.35	122.07
1	A	154	MSE	CG-SE-CE	-7.47	82.49	98.92
1	B	393	LYS	N-CA-C	-7.41	103.14	111.14
1	B	293	ASP	CA-C-N	-7.36	112.74	120.03
1	B	293	ASP	C-N-CA	-7.36	112.74	120.03
1	A	111	MSE	CG-SE-CE	7.30	114.99	98.92
1	A	302	MSE	N-CA-C	7.10	121.53	113.01
1	A	73	LEU	N-CA-C	-6.89	103.83	111.82
1	B	229	GLU	N-CA-C	-6.79	104.99	113.55
1	B	211	LEU	N-CA-C	-6.75	103.92	111.28
1	B	217	ALA	N-CA-C	-6.67	104.01	111.28
1	A	119	MSE	CG-SE-CE	6.66	113.57	98.92
1	A	119	MSE	N-CA-CB	-6.63	100.34	110.16
1	B	327	MSE	N-CA-CB	-6.56	99.78	109.95
1	B	71	PHE	N-CA-C	-6.49	102.46	111.81
1	A	119	MSE	N-CA-C	6.48	118.42	111.36
1	B	108	GLY	N-CA-C	6.45	123.93	115.36
1	B	178	THR	CA-C-N	-6.42	111.81	119.84
1	B	178	THR	C-N-CA	-6.42	111.81	119.84
1	B	46	ASN	N-CA-C	6.30	120.65	113.15
1	A	300	ILE	N-CA-C	6.26	122.35	109.34
1	B	388	LYS	N-CA-C	6.26	118.18	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	MSE	CG-SE-CE	-6.25	85.17	98.92
1	A	111	MSE	CA-CB-CG	6.23	126.55	114.10
1	B	303	THR	N-CA-C	6.22	119.79	109.46
1	B	144	GLU	N-CA-C	6.19	123.98	110.80
1	B	160	ALA	N-CA-C	-6.17	101.33	110.46
1	A	229	GLU	N-CA-C	-6.15	104.75	112.93
1	B	81	ALA	N-CA-C	-6.06	103.42	111.24
1	A	392	MSE	CG-SE-CE	5.98	112.08	98.92
1	B	151	PHE	N-CA-C	5.97	119.31	110.48
1	A	267	MSE	CB-CG-SE	5.92	130.46	112.70
1	B	407	LYS	N-CA-C	5.91	117.40	111.07
1	B	90	THR	N-CA-C	-5.90	106.32	112.93
1	B	103	MSE	N-CA-CB	-5.84	101.53	110.01
1	B	237	LYS	N-CA-C	5.83	118.16	109.59
1	B	302	MSE	CB-CG-SE	5.78	130.04	112.70
1	A	90	THR	N-CA-C	-5.74	106.33	113.15
1	B	102	HIS	N-CA-C	-5.72	105.02	112.23
1	A	266	MSE	N-CA-CB	-5.68	101.49	110.06
1	A	45	GLU	N-CA-C	5.67	122.89	110.80
1	A	292	ASN	N-CA-C	5.54	119.34	112.58
1	A	266	MSE	N-CA-C	5.53	118.93	110.20
1	A	294	PRO	N-CA-C	-5.49	102.49	111.21
1	B	130	ILE	N-CA-C	5.47	115.66	107.51
1	A	130	ILE	N-CA-C	5.38	115.60	107.80
1	B	105	LYS	N-CA-C	-5.38	105.32	111.07
1	B	99	LYS	N-CA-C	-5.36	104.33	111.24
1	B	266	MSE	N-CA-C	-5.34	101.27	109.76
1	A	98	ARG	N-CA-C	-5.32	106.63	113.23
1	B	45	GLU	N-CA-C	5.29	122.06	110.80
1	B	321	MSE	N-CA-CB	5.24	119.23	110.85
1	A	102	HIS	N-CA-C	-5.22	105.50	111.14
1	B	391	ALA	N-CA-C	5.21	116.76	111.14
1	B	280	THR	N-CA-C	-5.17	106.80	113.01
1	A	67	GLY	N-CA-C	-5.17	104.50	111.54
1	A	46	ASN	N-CA-C	5.12	118.67	112.93
1	A	217	ALA	N-CA-C	-5.12	105.82	111.71
1	A	268	TRP	N-CA-CB	-5.10	103.33	111.43
1	B	139	TRP	N-CA-C	-5.03	105.71	111.14
1	B	107	LEU	N-CA-C	-5.02	107.18	113.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	TYR	Sidechain

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	3125	0	3048	185	0
1	B	3096	0	3019	212	0
2	A	9	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	180	0	0	5	0
4	B	166	0	0	4	0
All	All	6578	0	6071	373	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 30.

All (373) 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:A:221:MSE:SE	1:B:190:MSE:HE1	1.36	1.74
1:A:165:GLN:HG2	1:A:190:MSE:CE	1.49	1.40
1:A:221:MSE:SE	1:B:190:MSE:CE	2.28	1.28
1:A:165:GLN:CG	1:A:190:MSE:CE	2.20	1.19
1:B:50:LEU:HD13	1:B:78:ARG:HB2	1.20	1.18
1:B:83:MSE:SE	1:B:107:LEU:HD21	1.94	1.15
1:B:50:LEU:HD22	1:B:78:ARG:HB3	1.30	1.11
1:B:60:GLU:HB2	1:B:75:MSE:HE1	1.32	1.11
1:A:165:GLN:CD	1:A:190:MSE:HE1	1.76	1.10
1:B:60:GLU:HB2	1:B:75:MSE:CE	1.81	1.10
1:A:80:MSE:HE1	1:A:107:LEU:HD13	1.20	1.08
1:A:165:GLN:HG2	1:A:190:MSE:HE2	1.09	1.06
1:A:42:THR:HG22	1:A:43:SER:H	1.15	1.06
1:A:80:MSE:HE1	1:A:107:LEU:CD1	1.86	1.05
1:B:72:THR:HG23	1:B:73:LEU:H	1.20	1.03
1:A:327:MSE:HE1	1:A:380:VAL:HG11	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:O	1:B:72:THR:HB	1.63	0.99
1:B:50:LEU:N	1:B:50:LEU:HD23	1.83	0.93
1:B:50:LEU:HD23	1:B:50:LEU:H	1.33	0.93
1:A:97:GLU:HG2	1:A:130:ILE:HD11	1.50	0.93
1:B:80:MSE:HE3	1:B:107:LEU:HD13	1.52	0.92
1:B:95:LEU:HB2	1:B:100:ILE:HD11	1.54	0.90
1:B:50:LEU:HD21	1:B:82:ARG:HH12	1.36	0.90
1:B:50:LEU:HD12	1:B:75:MSE:SE	2.22	0.90
1:B:166:GLN:HE21	1:B:187:PHE:HB3	1.37	0.89
1:B:50:LEU:HD13	1:B:78:ARG:CB	2.04	0.88
1:B:119:MSE:HE2	1:B:138:TRP:CZ3	2.10	0.87
1:B:138:TRP:O	1:B:141:SER:HB3	1.75	0.86
1:A:77:LYS:HD2	1:A:136:TRP:NE1	1.90	0.86
1:B:50:LEU:HD22	1:B:78:ARG:CB	2.06	0.86
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.41	0.86
1:A:131:THR:HG23	1:A:134:LYS:H	1.41	0.85
1:B:131:THR:HG23	1:B:134:LYS:H	1.41	0.84
1:B:88:ASP:OD1	1:B:92:LEU:HD23	1.77	0.84
1:A:165:GLN:CD	1:A:190:MSE:CE	2.44	0.83
1:B:60:GLU:HB2	1:B:75:MSE:HE2	1.64	0.80
1:A:42:THR:HG22	1:A:43:SER:N	1.96	0.79
1:A:131:THR:HG22	1:A:134:LYS:HB2	1.64	0.78
1:B:50:LEU:CD2	1:B:78:ARG:HB3	2.13	0.78
1:A:149:LYS:O	1:A:151:PHE:N	2.17	0.77
1:B:342:ARG:HD3	1:B:343:PHE:CZ	2.20	0.77
1:B:78:ARG:HG2	1:B:78:ARG:NH1	1.95	0.77
1:A:282:VAL:HG13	1:A:287:GLY:HA3	1.63	0.77
1:B:72:THR:HG23	1:B:73:LEU:N	1.97	0.76
1:B:60:GLU:CB	1:B:75:MSE:HE1	2.12	0.76
1:A:77:LYS:HD2	1:A:136:TRP:CD1	2.21	0.75
1:A:210:ASP:O	1:B:165:GLN:HG3	1.87	0.75
1:A:406:ARG:HH22	1:B:156:SER:HB3	1.54	0.73
1:A:149:LYS:C	1:A:151:PHE:H	1.96	0.73
1:A:165:GLN:CG	1:A:190:MSE:HE1	2.04	0.72
1:B:35:TYR:HA	1:B:60:GLU:HG2	1.70	0.72
1:A:165:GLN:CG	1:A:190:MSE:HE3	2.16	0.72
1:B:83:MSE:SE	1:B:107:LEU:CD2	2.84	0.72
1:A:283:VAL:HG21	1:A:401:MSE:HG2	1.70	0.71
1:A:184:LEU:HD13	1:A:197:GLN:NE2	2.05	0.70
1:A:33:ASN:OD1	1:A:61:PHE:HB3	1.92	0.70
1:A:42:THR:CG2	1:A:43:SER:H	1.96	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:MSE:HG2	1:B:123:ILE:HD12	1.73	0.69
1:A:35:TYR:OH	1:A:44:LEU:HD23	1.92	0.69
1:B:92:LEU:HD23	1:B:92:LEU:H	1.58	0.69
1:B:78:ARG:HH11	1:B:78:ARG:CG	2.06	0.68
1:B:342:ARG:HD3	1:B:343:PHE:CE2	2.27	0.68
1:A:166:GLN:HE21	1:A:187:PHE:HB3	1.59	0.68
1:A:288:TYR:CE2	1:A:327:MSE:HE3	2.29	0.68
1:A:221:MSE:HE2	4:A:697:HOH:O	1.93	0.68
1:B:322:ILE:HD11	1:B:380:VAL:HG13	1.76	0.67
1:B:50:LEU:HD21	1:B:82:ARG:NH1	2.08	0.66
1:A:52:GLU:HA	1:A:55:LYS:HE3	1.77	0.66
1:B:77:LYS:HD3	1:B:78:ARG:HH21	1.60	0.66
1:B:342:ARG:NE	4:B:1001:HOH:O	2.10	0.66
1:A:109:ARG:HG3	1:A:144:GLU:CD	2.21	0.66
1:B:122:GLU:CD	1:B:142:HIS:HE2	2.04	0.66
1:A:209:ARG:HD3	1:B:165:GLN:OE1	1.96	0.65
1:B:111:MSE:HE1	1:B:119:MSE:CE	2.25	0.65
1:A:405:LEU:O	1:A:405:LEU:HD12	1.97	0.65
1:A:38:THR:HB	1:A:83:MSE:SE	2.47	0.65
1:A:161:VAL:HG23	1:A:161:VAL:O	1.97	0.65
1:A:118:GLN:O	1:A:122:GLU:HG2	1.96	0.65
1:B:44:LEU:HD23	1:B:45:GLU:N	2.12	0.65
1:A:171:ARG:NH2	1:A:195:GLU:OE1	2.28	0.64
1:B:80:MSE:HE1	1:B:139:TRP:CE2	2.32	0.64
1:A:283:VAL:CG2	1:A:401:MSE:HG2	2.27	0.64
1:B:80:MSE:SE	1:B:136:TRP:HZ3	2.30	0.64
1:A:69:ASP:O	4:A:601:HOH:O	2.14	0.64
1:A:184:LEU:HD13	1:A:197:GLN:HE22	1.63	0.63
1:A:402:TRP:CZ2	1:A:406:ARG:HD2	2.33	0.63
1:B:111:MSE:HE1	1:B:119:MSE:HE3	1.81	0.63
1:B:282:VAL:O	1:B:289:VAL:HA	1.98	0.63
1:B:104:CYS:SG	1:B:119:MSE:HE1	2.38	0.63
1:A:340:ILE:HD11	1:A:354:LEU:HD11	1.81	0.63
1:B:322:ILE:N	1:B:322:ILE:HD12	2.13	0.63
1:B:35:TYR:OH	1:B:44:LEU:HG	1.98	0.62
1:B:95:LEU:HB2	1:B:100:ILE:CD1	2.27	0.62
1:B:100:ILE:HG13	1:B:130:ILE:HD12	1.82	0.62
1:B:50:LEU:H	1:B:50:LEU:CD2	1.97	0.62
1:B:281:ASP:O	1:B:282:VAL:HG23	2.00	0.61
1:A:55:LYS:HD2	1:A:56:ARG:HG3	1.82	0.61
1:A:414:VAL:HG11	4:A:742:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PRO:HG2	1:A:147:ALA:H	1.66	0.61
1:B:50:LEU:CD1	1:B:78:ARG:HB2	2.14	0.60
1:A:110:VAL:HG23	1:A:110:VAL:O	2.01	0.60
1:A:157:VAL:HG23	1:B:196:LEU:HD13	1.84	0.59
1:B:124:ASN:N	1:B:134:LYS:HZ3	2.00	0.59
1:B:77:LYS:HG3	1:B:136:TRP:CE2	2.37	0.59
1:B:69:ASP:O	1:B:72:THR:CB	2.45	0.59
1:A:245:PRO:O	1:A:246:PHE:HB2	2.02	0.59
1:B:119:MSE:HE2	1:B:138:TRP:HZ3	1.65	0.59
1:B:90:THR:OG1	1:B:92:LEU:HD22	2.03	0.59
1:B:109:ARG:HD2	1:B:139:TRP:CZ3	2.37	0.59
1:B:109:ARG:HD3	1:B:144:GLU:HG3	1.84	0.59
1:A:391:ALA:O	1:A:395:ILE:HG13	2.03	0.58
1:B:56:ARG:O	1:B:57:ASN:HB2	2.02	0.58
1:B:191:GLU:HA	1:B:191:GLU:OE2	2.04	0.58
1:A:49:PRO:HG2	1:A:54:CYS:SG	2.42	0.58
1:B:284:PHE:O	1:B:286:GLY:N	2.36	0.58
1:B:351:PRO:HG3	1:B:358:LEU:HD12	1.86	0.58
1:A:78:ARG:HH11	1:A:78:ARG:HB2	1.68	0.58
1:A:208:VAL:HB	1:A:223:ARG:HG2	1.85	0.58
1:A:289:VAL:HG22	1:A:289:VAL:O	2.03	0.58
1:A:131:THR:CG2	1:A:134:LYS:H	2.15	0.58
1:A:406:ARG:NH2	1:B:156:SER:HB3	2.19	0.58
1:B:165:GLN:CD	1:B:190:MSE:SE	2.97	0.57
1:B:177:TYR:HD1	1:B:251:GLN:HE22	1.51	0.57
1:A:251:GLN:HG2	1:A:253:ILE:HD11	1.86	0.57
1:B:50:LEU:HB2	1:B:75:MSE:SE	2.54	0.57
1:B:70:GLU:C	1:B:72:THR:H	2.10	0.57
1:A:283:VAL:HG22	1:A:284:PHE:HD1	1.69	0.57
1:A:324:ASP:CG	1:A:324:ASP:O	2.48	0.57
1:B:145:VAL:HG23	1:B:145:VAL:O	2.03	0.57
1:B:183:VAL:HB	1:B:249:ILE:HB	1.87	0.56
1:A:114:ASP:HA	1:A:117:LYS:HE3	1.87	0.56
1:A:276:THR:HB	1:A:398:SER:OG	2.04	0.56
1:A:241:ALA:HB2	1:A:250:LYS:HG2	1.86	0.56
1:B:119:MSE:O	1:B:123:ILE:HG13	2.04	0.56
1:B:324:ASP:CG	1:B:324:ASP:O	2.48	0.56
1:A:298:ILE:HD11	1:A:365:PHE:CE2	2.40	0.56
1:B:104:CYS:HB3	1:B:111:MSE:HE3	1.87	0.56
1:A:380:VAL:HG23	1:A:381:PHE:HD1	1.71	0.56
1:A:284:PHE:HZ	1:A:397:GLU:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:HIS:C	1:A:144:GLU:H	2.13	0.56
1:B:359:ASP:OD1	4:B:1002:HOH:O	2.18	0.56
1:B:35:TYR:HA	1:B:60:GLU:CG	2.36	0.56
1:A:80:MSE:HE1	1:A:107:LEU:HD11	1.86	0.55
1:B:50:LEU:HD12	1:B:75:MSE:CE	2.37	0.55
1:A:123:ILE:O	1:A:124:ASN:C	2.50	0.55
1:A:192:THR:OG1	1:A:194:LYS:HG2	2.07	0.55
1:B:208:VAL:HB	1:B:223:ARG:HG2	1.88	0.55
1:B:209:ARG:HE	1:B:221:MSE:HE1	1.72	0.55
1:A:52:GLU:CD	1:A:52:GLU:H	2.13	0.55
1:A:143:PRO:O	1:A:144:GLU:O	2.25	0.55
1:A:146:PRO:HG2	1:A:147:ALA:N	2.22	0.54
1:A:254:LYS:HD3	1:A:259:ARG:HH11	1.71	0.54
1:B:35:TYR:HB3	1:B:60:GLU:CD	2.32	0.54
1:A:80:MSE:SE	1:B:255:ASN:C	3.01	0.54
1:A:152:PHE:HB2	1:A:154:MSE:HE3	1.89	0.54
1:B:359:ASP:OD1	1:B:359:ASP:N	2.40	0.54
1:B:106:TYR:C	1:B:108:GLY:H	2.15	0.54
1:A:152:PHE:O	1:A:154:MSE:HG2	2.08	0.54
1:A:175:GLU:HB3	1:A:178:THR:CG2	2.38	0.54
1:B:232:LYS:HE3	1:B:233:TRP:CZ2	2.42	0.54
1:B:283:VAL:HA	1:B:288:TYR:O	2.07	0.54
1:A:283:VAL:HG22	1:A:284:PHE:CD1	2.44	0.53
1:B:109:ARG:NH1	1:B:139:TRP:CE3	2.76	0.53
1:B:157:VAL:HG13	1:B:158:ASP:N	2.21	0.53
1:B:92:LEU:H	1:B:92:LEU:CD2	2.22	0.53
1:B:124:ASN:N	1:B:134:LYS:NZ	2.56	0.53
1:A:148:LYS:HA	1:A:148:LYS:NZ	2.23	0.53
1:B:50:LEU:N	1:B:50:LEU:CD2	2.54	0.53
1:B:73:LEU:HD12	1:B:73:LEU:O	2.08	0.53
1:A:141:SER:C	1:A:142:HIS:ND1	2.67	0.53
1:A:290:GLY:O	1:A:326:GLN:HG2	2.08	0.53
1:B:80:MSE:HE3	1:B:107:LEU:CD1	2.33	0.53
1:A:144:GLU:O	1:A:145:VAL:O	2.27	0.52
1:A:284:PHE:CZ	1:A:397:GLU:HB3	2.44	0.52
1:B:50:LEU:CD2	1:B:82:ARG:HH12	2.14	0.52
1:B:72:THR:CG2	1:B:73:LEU:H	1.99	0.52
1:B:259:ARG:HD3	4:B:1072:HOH:O	2.08	0.52
1:B:318:ILE:HD11	1:B:329:TRP:HB3	1.90	0.52
1:A:262:LYS:HE2	1:B:67:GLY:O	2.08	0.52
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:MSE:O	1:B:104:CYS:C	2.42	0.52
1:A:162:PRO:O	1:A:163:TYR:HB3	2.09	0.52
1:A:159:PHE:CE1	1:A:161:VAL:HG11	2.44	0.52
1:B:186:TYR:CE1	1:B:197:GLN:HG3	2.45	0.52
1:A:49:PRO:O	1:A:50:LEU:C	2.53	0.52
1:A:52:GLU:HG3	1:A:75:MSE:SE	2.60	0.52
1:A:145:VAL:HB	1:A:148:LYS:CB	2.40	0.52
1:A:149:LYS:HB3	1:A:149:LYS:NZ	2.25	0.52
1:B:35:TYR:CB	1:B:60:GLU:CD	2.83	0.51
1:B:245:PRO:O	1:B:246:PHE:HB2	2.09	0.51
1:A:296:ASP:OD1	4:A:602:HOH:O	2.18	0.51
1:B:50:LEU:HD12	1:B:75:MSE:HA	1.92	0.51
1:A:221:MSE:HE3	1:B:165:GLN:HE22	1.76	0.51
1:B:77:LYS:CD	1:B:78:ARG:NH2	2.74	0.51
1:B:158:ASP:OD1	1:B:159:PHE:N	2.44	0.51
1:A:176:LEU:O	1:A:177:TYR:HB2	2.11	0.51
1:A:78:ARG:HB2	1:A:78:ARG:NH1	2.25	0.50
1:A:182:ARG:HA	1:A:249:ILE:O	2.10	0.50
1:A:348:HIS:O	1:A:351:PRO:HD2	2.10	0.50
1:A:358:LEU:HB3	1:A:385:PHE:CE2	2.47	0.50
1:B:176:LEU:O	1:B:177:TYR:HB2	2.11	0.50
1:A:406:ARG:HA	1:B:154:MSE:HE2	1.93	0.50
1:A:253:ILE:HD13	1:A:258:PRO:HA	1.93	0.50
1:A:68:LYS:NZ	1:B:262:LYS:O	2.41	0.50
1:A:163:TYR:HE2	1:A:211:LEU:HD22	1.75	0.50
1:B:80:MSE:HE1	1:B:139:TRP:CD2	2.47	0.50
1:B:291:ASP:O	1:B:292:ASN:HB2	2.11	0.50
1:B:118:GLN:O	1:B:122:GLU:HG3	2.12	0.49
1:B:145:VAL:HG23	1:B:148:LYS:HE3	1.93	0.49
1:B:189:ASP:OD1	1:B:191:GLU:HB2	2.12	0.49
1:A:52:GLU:CG	1:A:75:MSE:HE3	2.41	0.49
1:B:119:MSE:HG2	1:B:123:ILE:CD1	2.42	0.49
1:B:269:ASN:ND2	1:B:305:PHE:H	2.10	0.49
1:A:175:GLU:HB3	1:A:178:THR:HG21	1.95	0.49
1:B:56:ARG:O	1:B:57:ASN:CB	2.60	0.49
1:B:122:GLU:CD	1:B:138:TRP:HE1	2.19	0.49
1:A:113:GLU:O	1:A:117:LYS:HG3	2.13	0.49
1:A:412:GLU:CG	1:A:413:GLU:N	2.75	0.49
1:B:133:GLU:OE2	1:B:133:GLU:HA	2.12	0.49
1:B:252:ASP:C	1:B:252:ASP:OD1	2.56	0.49
1:A:50:LEU:HG	1:A:60:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HG23	1:B:134:LYS:HE3	1.95	0.49
1:B:189:ASP:OD1	1:B:191:GLU:CB	2.61	0.48
1:A:342:ARG:HD2	1:A:342:ARG:O	2.12	0.48
1:B:114:ASP:O	1:B:117:LYS:HB2	2.13	0.48
1:A:221:MSE:CE	1:B:165:GLN:HE22	2.25	0.48
1:A:288:TYR:CZ	1:A:327:MSE:CE	2.96	0.48
1:A:64:VAL:O	1:B:262:LYS:NZ	2.46	0.48
1:A:284:PHE:CD1	1:A:284:PHE:N	2.82	0.48
1:B:77:LYS:CD	1:B:78:ARG:HH21	2.25	0.48
1:A:157:VAL:O	1:A:158:ASP:C	2.56	0.48
1:B:77:LYS:HD3	1:B:78:ARG:NH2	2.27	0.48
1:B:369:LYS:NZ	1:B:377:ASN:HD21	2.11	0.48
1:A:251:GLN:HG2	1:A:253:ILE:CD1	2.43	0.48
1:B:145:VAL:CG2	1:B:148:LYS:HE3	2.44	0.48
1:B:94:TYR:CD1	1:B:94:TYR:C	2.92	0.47
1:A:97:GLU:HG2	1:A:130:ILE:CD1	2.32	0.47
1:A:318:ILE:HD11	1:A:329:TRP:HB3	1.96	0.47
1:B:44:LEU:CD2	1:B:45:GLU:N	2.76	0.47
1:B:48:LYS:HB2	1:B:48:LYS:NZ	2.28	0.47
1:B:282:VAL:HG21	1:B:401:MSE:SE	2.64	0.47
1:A:390:PHE:O	1:A:394:VAL:HG23	2.14	0.47
1:A:412:GLU:HG3	1:A:413:GLU:N	2.28	0.47
1:B:110:VAL:HG23	1:B:110:VAL:O	2.15	0.47
1:A:90:THR:O	1:A:91:GLN:C	2.58	0.47
1:A:152:PHE:HZ	1:B:292:ASN:ND2	2.13	0.47
1:A:153:SER:OG	1:B:245:PRO:HA	2.14	0.47
1:B:61:PHE:CD1	1:B:61:PHE:C	2.92	0.47
1:A:120:LYS:O	1:A:124:ASN:N	2.42	0.47
1:A:362:HIS:C	1:A:362:HIS:CD2	2.93	0.47
1:A:146:PRO:CG	1:A:147:ALA:N	2.78	0.46
1:B:166:GLN:NE2	1:B:187:PHE:HB3	2.19	0.46
1:A:90:THR:O	1:A:92:LEU:HG	2.15	0.46
1:A:35:TYR:HA	1:A:60:GLU:HB2	1.97	0.46
1:A:94:TYR:CD1	1:A:94:TYR:C	2.93	0.46
1:A:299:GLU:CD	1:A:301:GLY:H	2.22	0.46
1:A:406:ARG:HE	1:B:154:MSE:HE3	1.79	0.46
1:A:149:LYS:C	1:A:149:LYS:HD2	2.41	0.46
1:B:50:LEU:CD2	1:B:82:ARG:NH1	2.77	0.46
1:A:289:VAL:HG22	1:A:326:GLN:HA	1.98	0.46
1:A:99:LYS:HA	1:A:99:LYS:HD3	1.65	0.46
1:A:80:MSE:SE	1:B:255:ASN:O	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ARG:HG3	1:B:188:ARG:HH11	1.81	0.46
1:A:149:LYS:HE2	1:B:292:ASN:HD22	1.80	0.45
1:B:284:PHE:O	1:B:285:GLU:C	2.58	0.45
1:B:50:LEU:CD1	1:B:78:ARG:CB	2.87	0.45
1:B:176:LEU:O	1:B:177:TYR:CB	2.65	0.45
1:A:144:GLU:O	1:A:145:VAL:C	2.58	0.45
1:A:145:VAL:HB	1:A:148:LYS:HB3	1.98	0.45
1:A:189:ASP:O	1:A:193:GLY:N	2.47	0.45
1:B:406:ARG:HA	1:B:406:ARG:HD2	1.58	0.45
1:A:288:TYR:CZ	1:A:327:MSE:HE3	2.50	0.45
1:A:136:TRP:CZ2	1:A:140:CYS:SG	3.10	0.45
1:B:50:LEU:CD1	1:B:75:MSE:CE	2.95	0.45
1:A:177:TYR:N	1:A:251:GLN:OE1	2.44	0.45
1:B:56:ARG:HE	1:B:56:ARG:HB3	1.44	0.45
1:A:52:GLU:HG3	1:A:75:MSE:CE	2.47	0.45
1:A:227:ILE:O	1:A:271:GLY:HA3	2.17	0.45
1:B:188:ARG:NH1	1:B:195:GLU:OE2	2.50	0.44
1:A:321:MSE:SE	1:A:365:PHE:HB3	2.67	0.44
1:B:35:TYR:HB2	1:B:60:GLU:OE1	2.16	0.44
1:B:52:GLU:OE2	1:B:74:SER:OG	2.34	0.44
1:A:131:THR:CG2	1:A:134:LYS:HB2	2.43	0.44
1:A:36:ILE:N	1:A:36:ILE:HD13	2.32	0.44
1:A:165:GLN:HB3	1:A:190:MSE:HE3	2.00	0.44
1:A:166:GLN:HG2	1:B:159:PHE:HE2	1.82	0.44
1:B:88:ASP:CA	1:B:95:LEU:HD21	2.48	0.44
1:B:254:LYS:O	1:B:255:ASN:HB2	2.17	0.44
1:B:50:LEU:HG	1:B:75:MSE:HE1	2.00	0.44
1:B:124:ASN:H	1:B:134:LYS:NZ	2.15	0.44
1:A:145:VAL:HB	1:A:148:LYS:HB2	1.99	0.44
1:B:299:GLU:HA	1:B:333:CYS:O	2.18	0.44
1:A:78:ARG:HH11	1:A:78:ARG:CB	2.31	0.43
1:A:164:HIS:HD2	1:A:189:ASP:OD2	2.01	0.43
1:B:106:TYR:C	1:B:108:GLY:N	2.75	0.43
1:A:78:ARG:O	1:A:82:ARG:HG3	2.18	0.43
1:B:119:MSE:CG	1:B:123:ILE:CD1	2.96	0.43
1:B:165:GLN:HG2	1:B:190:MSE:SE	2.68	0.43
1:B:316:LEU:O	1:B:347:ILE:HB	2.18	0.43
1:B:42:THR:HB	1:B:43:SER:H	1.56	0.43
1:B:44:LEU:O	1:B:47:VAL:HG22	2.18	0.43
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.88	0.43
1:A:164:HIS:CD2	1:A:189:ASP:OD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ILE:HG13	1:B:335:SER:N	2.31	0.43
1:B:277:TRP:O	1:B:401:MSE:HE3	2.17	0.43
1:A:354:LEU:O	1:A:355:PRO:C	2.59	0.43
1:A:388:LYS:O	1:A:392:MSE:HG3	2.19	0.43
1:B:92:LEU:CD2	1:B:92:LEU:N	2.82	0.43
1:B:112:ASN:O	1:B:113:GLU:C	2.61	0.43
1:B:186:TYR:HA	1:B:196:LEU:O	2.19	0.43
1:B:321:MSE:C	1:B:322:ILE:HD12	2.44	0.43
1:A:257:VAL:HG21	1:B:76:GLU:HG2	1.99	0.43
1:B:89:VAL:C	1:B:91:GLN:H	2.27	0.43
1:B:113:GLU:O	1:B:117:LYS:HG2	2.19	0.43
1:B:119:MSE:HG3	1:B:123:ILE:HD11	2.00	0.43
1:B:405:LEU:HD12	1:B:405:LEU:O	2.19	0.43
1:A:42:THR:CG2	1:A:43:SER:N	2.67	0.42
1:A:283:VAL:CG2	1:A:284:PHE:HD1	2.32	0.42
1:B:70:GLU:C	1:B:72:THR:N	2.77	0.42
1:A:200:PRO:HA	1:A:204:ILE:CD1	2.49	0.42
1:B:72:THR:CG2	1:B:73:LEU:N	2.68	0.42
1:A:110:VAL:HG22	1:A:144:GLU:OE2	2.18	0.42
1:A:167:GLN:OE1	1:B:213:ARG:HD3	2.19	0.42
1:A:118:GLN:HE22	1:A:142:HIS:CD2	2.38	0.42
1:B:50:LEU:CD1	1:B:75:MSE:HA	2.48	0.42
1:B:50:LEU:CD1	1:B:75:MSE:SE	3.08	0.42
1:A:165:GLN:CB	1:A:190:MSE:HE3	2.49	0.42
1:A:209:ARG:HG2	1:A:221:MSE:HE1	2.01	0.42
1:B:77:LYS:HD2	1:B:78:ARG:NH2	2.34	0.42
1:B:35:TYR:CE1	1:B:47:VAL:HG21	2.54	0.42
1:B:184:LEU:HD23	1:B:248:PRO:HB3	2.02	0.42
1:A:38:THR:HA	1:A:83:MSE:HE1	2.01	0.42
1:B:131:THR:OG1	1:B:132:PHE:N	2.53	0.42
1:A:52:GLU:HG3	1:A:75:MSE:HE3	2.01	0.42
1:B:211:LEU:H	1:B:211:LEU:HG	1.58	0.42
1:B:46:ASN:ND2	4:B:1012:HOH:O	2.52	0.42
1:B:78:ARG:HD3	1:B:78:ARG:HA	1.81	0.42
1:A:277:TRP:CD2	1:A:405:LEU:HD22	2.55	0.41
1:A:148:LYS:HA	1:A:148:LYS:HZ3	1.83	0.41
1:A:405:LEU:HD12	1:A:405:LEU:C	2.45	0.41
1:A:198:VAL:HG12	1:B:157:VAL:HB	2.02	0.41
1:B:393:LYS:HA	1:B:396:ASP:OD2	2.20	0.41
1:A:157:VAL:CG2	1:B:196:LEU:HD13	2.50	0.41
1:B:158:ASP:O	1:B:159:PHE:HB2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HH21	1:B:342:ARG:HG3	1.85	0.41
1:B:50:LEU:HD12	1:B:75:MSE:HE3	2.02	0.41
1:A:52:GLU:HA	1:A:55:LYS:CE	2.47	0.41
1:B:229:GLU:O	1:B:238:PHE:HB2	2.21	0.41
1:A:50:LEU:HB3	1:A:52:GLU:OE2	2.21	0.41
1:A:156:SER:C	1:A:158:ASP:N	2.77	0.41
1:B:33:ASN:ND2	1:B:33:ASN:O	2.54	0.41
1:B:44:LEU:CD2	1:B:45:GLU:H	2.33	0.41
1:B:129:HIS:N	1:B:129:HIS:CD2	2.87	0.41
1:A:89:VAL:C	1:A:91:GLN:H	2.28	0.41
1:B:322:ILE:N	1:B:322:ILE:CD1	2.82	0.41
1:B:269:ASN:HD21	1:B:305:PHE:H	1.68	0.40
1:A:58:VAL:HA	4:A:637:HOH:O	2.22	0.40
1:A:241:ALA:HB1	1:A:244:GLU:HG3	2.02	0.40
1:A:409:ASN:OD1	1:A:409:ASN:N	2.54	0.40
1:B:358:LEU:HB3	1:B:385:PHE:CE2	2.56	0.40
1:A:236:ALA:HA	1:A:260:PHE:CD1	2.56	0.40
1:A:277:TRP:CE2	1:A:405:LEU:HD22	2.56	0.40
1:A:97:GLU:OE2	1:A:120:LYS:HE2	2.22	0.40
1:A:146:PRO:CG	1:A:147:ALA:H	2.23	0.40
1:A:232:LYS:O	1:A:233:TRP:HB2	2.21	0.40
1:B:50:LEU:CD1	1:B:75:MSE:HE3	2.52	0.40
1:B:100:ILE:H	1:B:100:ILE:HG12	1.73	0.40
1:B:140:CYS:C	1:B:141:SER:O	2.64	0.40
1:A:215:LYS:H	1:A:215:LYS:HG3	1.65	0.40
1:B:188:ARG:HG3	1:B:188:ARG:NH1	2.36	0.40
1:B:320:GLY:HA3	1:B:380:VAL:CG2	2.51	0.40
1:B:347:ILE:HD12	1:B:347:ILE:HA	1.92	0.40
1:B:391:ALA:O	1:B:395:ILE:HG13	2.22	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	380/414 (92%)	344 (90%)	26 (7%)	10 (3%)	4	6
1	B	377/414 (91%)	331 (88%)	31 (8%)	15 (4%)	2	2
All	All	757/828 (91%)	675 (89%)	57 (8%)	25 (3%)	3	4

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	44	LEU
1	A	45	GLU
1	A	144	GLU
1	A	145	VAL
1	A	146	PRO
1	A	150	ASP
1	B	44	LEU
1	B	45	GLU
1	B	144	GLU
1	B	147	ALA
1	B	285	GLU
1	B	141	SER
1	B	150	ASP
1	A	147	ALA
1	A	285	GLU
1	B	143	PRO
1	B	159	PHE
1	A	91	GLN
1	B	72	THR
1	B	97	GLU
1	B	124	ASN
1	B	145	VAL
1	B	282	VAL
1	B	57	ASN

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	340/347 (98%)	310 (91%)	30 (9%)	9	19
1	B	336/347 (97%)	300 (89%)	36 (11%)	6	13
All	All	676/694 (97%)	610 (90%)	66 (10%)	7	15

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	44	LEU
1	A	52	GLU
1	A	55	LYS
1	A	58	VAL
1	A	74	SER
1	A	89	VAL
1	A	91	GLN
1	A	98	ARG
1	A	100	ILE
1	A	114	ASP
1	A	118	GLN
1	A	123	ILE
1	A	126	ILE
1	A	134	LYS
1	A	145	VAL
1	A	148	LYS
1	A	149	LYS
1	A	184	LEU
1	A	195	GLU
1	A	239	GLU
1	A	250	LYS
1	A	266	MSE
1	A	283	VAL
1	A	284	PHE
1	A	288	TYR
1	A	289	VAL
1	A	324	ASP
1	A	342	ARG
1	A	404	ASN
1	B	42	THR
1	B	46	ASN
1	B	48	LYS
1	B	50	LEU
1	B	52	GLU

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Mol	Chain	Res	Type
1	B	55	LYS
1	B	78	ARG
1	B	92	LEU
1	B	96	GLU
1	B	101	GLU
1	B	112	ASN
1	B	121	SER
1	B	124	ASN
1	B	126	ILE
1	B	150	ASP
1	B	157	VAL
1	B	161	VAL
1	B	170	THR
1	B	188	ARG
1	B	191	GLU
1	B	194	LYS
1	B	209	ARG
1	B	221	MSE
1	B	282	VAL
1	B	283	VAL
1	B	302	MSE
1	B	321	MSE
1	B	324	ASP
1	B	334	ILE
1	B	339	PRO
1	B	342	ARG
1	B	359	ASP
1	B	367	VAL
1	B	378	LYS
1	B	396	ASP
1	B	408	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	164	HIS
1	A	166	GLN
1	A	263	HIS
1	A	362	HIS
1	A	377	ASN
1	A	382	ASN

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Mol	Chain	Res	Type
1	B	33	ASN
1	B	46	ASN
1	B	124	ASN
1	B	166	GLN
1	B	269	ASN
1	B	372	GLN
1	B	377	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLT	A	501	-	8,8,8	1.16	1 (12%)	10,10,10	1.63	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLT	A	501	-	-	0/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MLT	O2-C1	-2.45	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MLT	O2-C1-C2	3.47	120.07	112.74
2	A	501	MLT	O2-C1-O1	-2.08	119.37	124.08

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 [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	366/414 (88%)	-0.44	3 (0%) 82 80	13, 35, 76, 89	0
1	B	363/414 (87%)	-0.20	15 (4%) 41 36	13, 34, 105, 143	0
All	All	729/828 (88%)	-0.32	18 (2%) 58 53	13, 34, 95, 143	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	PRO	4.5
1	B	49	PRO	3.7
1	B	53	ALA	3.4
1	B	44	LEU	3.0
1	A	414	VAL	3.0
1	B	52	GLU	2.9
1	B	36	ILE	2.9
1	B	50	LEU	2.8
1	B	43	SER	2.8
1	B	38	THR	2.8
1	B	37	GLY	2.7
1	B	39	GLY	2.7
1	A	147	ALA	2.5
1	B	126	ILE	2.4
1	B	110	VAL	2.3
1	B	40	LEU	2.2
1	B	48	LYS	2.0
1	A	283	VAL	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](#)

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
3	MG	A	502	1/1	0.84	0.18	41,41,41,41	0
3	MG	B	900	1/1	0.86	0.18	53,53,53,53	0
2	MLT	A	501	9/9	0.94	0.08	56,57,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.