



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:51 PM UTC

PDB ID : 5H0T / pdb_00005h0t
Title : Crystal structure of proliferating cell nuclear antigen from Leishmania donovani at 2.73 Angstrom resolution
Authors : Singh, P.K.; Yadav, S.P.; Sharma, P.S.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-10-06
Resolution : 2.73 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

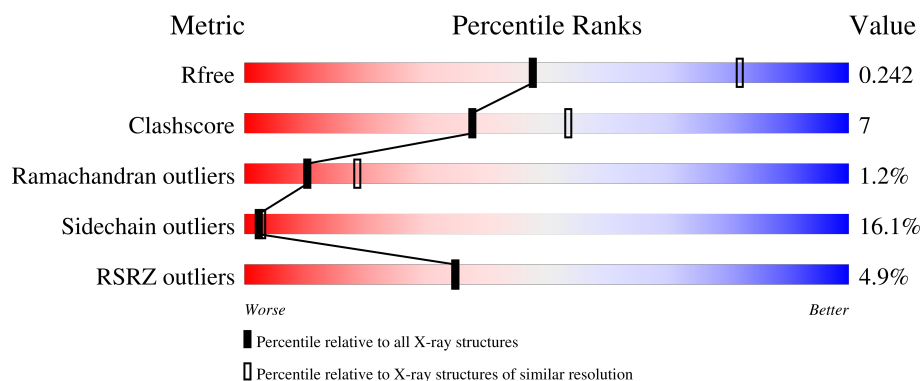
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	292	3% 62% 17% 5% 15%
1	B	292	4% 63% 17% • 15%
1	C	292	6% 59% 20% 5% • 15%
1	D	292	3% 61% 20% • • 15%
1	E	292	3% 63% 15% 5% • 15%

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Mol	Chain	Length	Quality of chain
1	F	292	6% 61% 19% • • 15%

2 Entry composition [i](#)

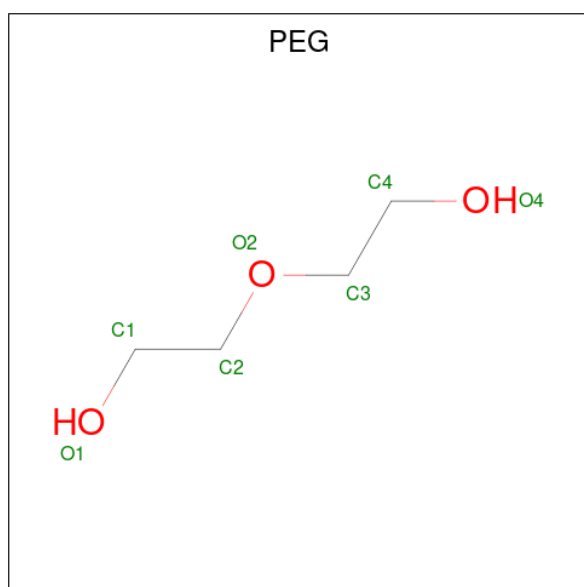
There are 3 unique types of molecules in this entry. The entry contains 11778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	D	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	E	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	B	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	C	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			
1	F	248	Total	C	N	O	S	0	0	0
			1919	1210	317	377	15			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		

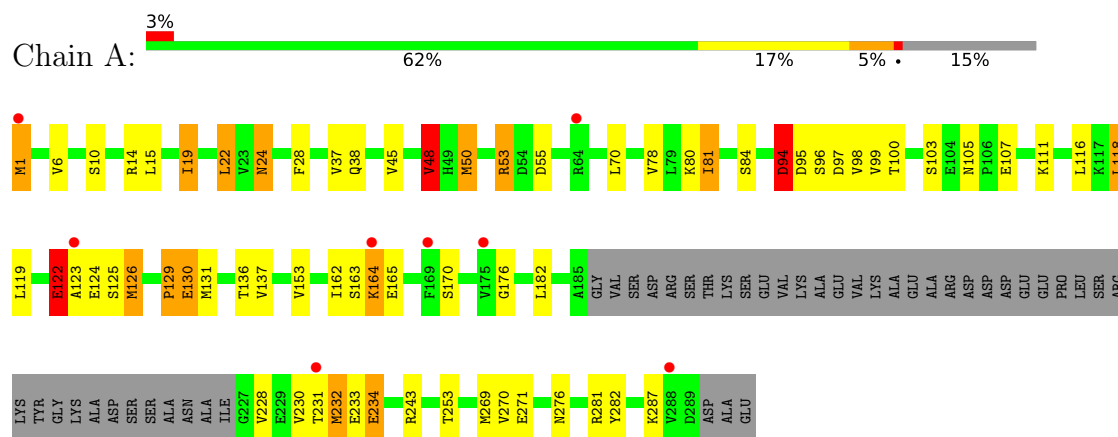
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	D	59	Total	O	0	0
			59	59		
3	E	53	Total	O	0	0
			53	53		
3	B	26	Total	O	0	0
			26	26		
3	C	30	Total	O	0	0
			30	30		
3	F	27	Total	O	0	0
			27	27		

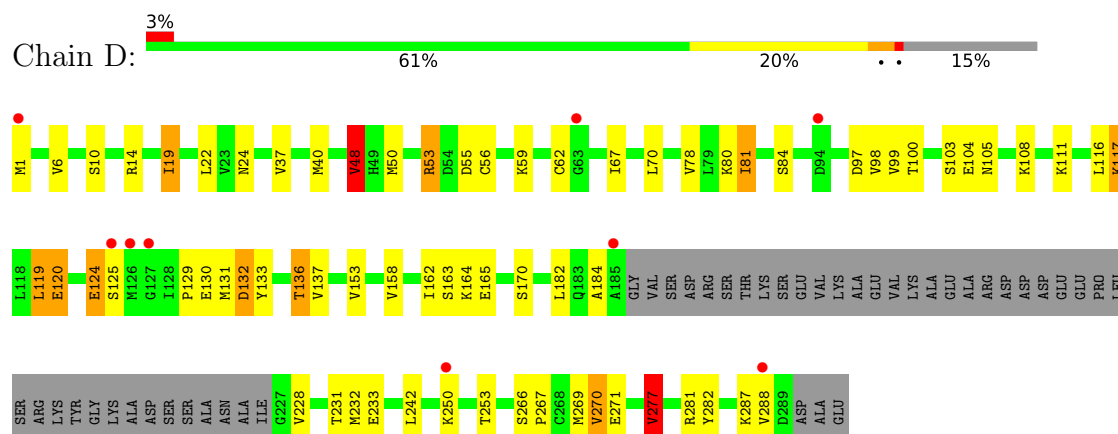
3 Residue-property plots [i](#)

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.

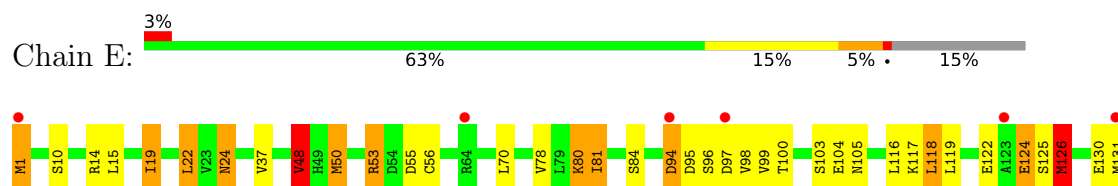
- Molecule 1: Proliferating cell nuclear antigen

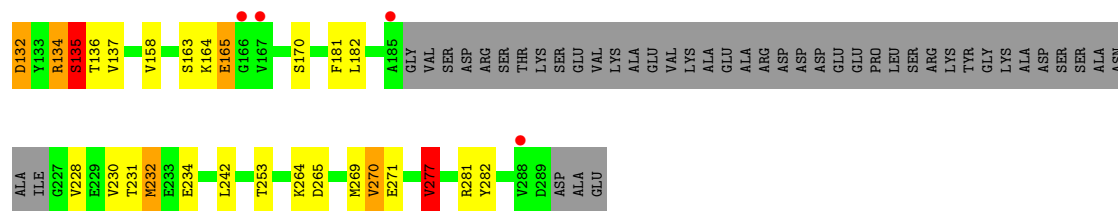


- Molecule 1: Proliferating cell nuclear antigen

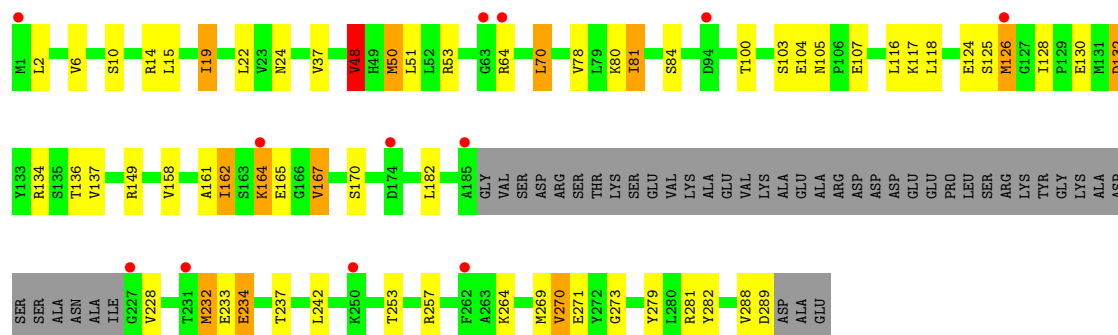


- Molecule 1: Proliferating cell nuclear antigen

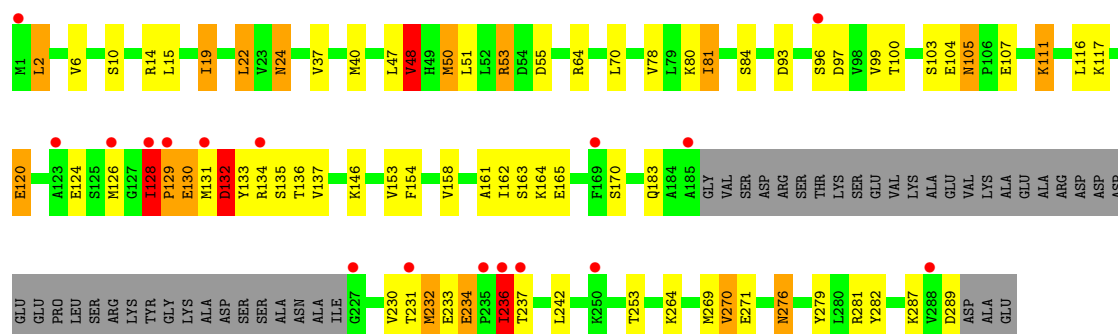




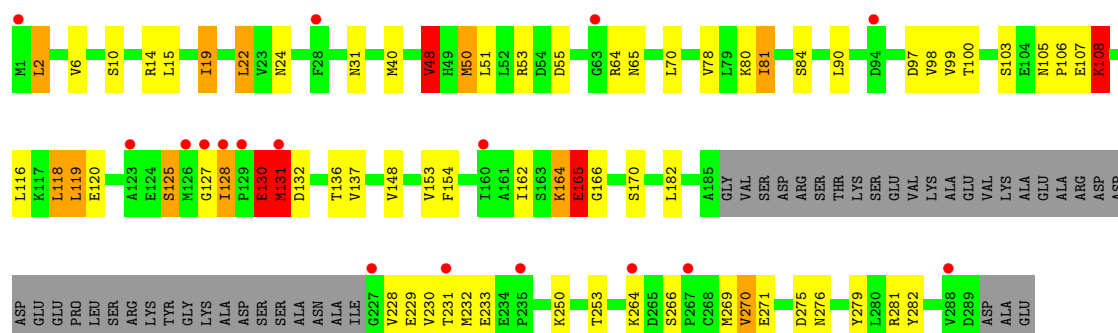
• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen



• Molecule 1: Proliferating cell nuclear antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.80Å 149.57Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.08 – 2.73 112.08 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (112.08-2.73) 99.5 (112.08-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.197 , 0.239 0.202 , 0.242	Depositor DCC
R_{free} test set	927 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11778	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: PEG

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	1.25	6/1947 (0.3%)	1.32	13/2627 (0.5%)
1	B	1.15	2/1947 (0.1%)	1.24	11/2627 (0.4%)
1	C	1.21	3/1947 (0.2%)	1.27	9/2627 (0.3%)
1	D	1.18	3/1947 (0.2%)	1.30	16/2627 (0.6%)
1	E	1.17	2/1947 (0.1%)	1.25	12/2627 (0.5%)
1	F	1.15	5/1947 (0.3%)	1.30	18/2627 (0.7%)
All	All	1.18	21/11682 (0.2%)	1.28	79/15762 (0.5%)

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	2
1	B	0	2
1	C	0	2
1	D	0	1
1	F	0	3
All	All	0	10

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	287	LYS	C-O	-8.30	1.13	1.24
1	A	45	VAL	C-O	-7.32	1.16	1.24
1	E	119	LEU	CA-C	-6.24	1.45	1.52
1	B	273	GLY	C-O	-6.21	1.18	1.24
1	D	62	CYS	C-O	6.16	1.32	1.23
1	A	1	MET	N-CA	6.09	1.57	1.46
1	C	2	LEU	N-CA	5.64	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	GLY	C-O	-5.62	1.19	1.23
1	B	128	ILE	CA-C	5.54	1.58	1.52
1	F	119	LEU	C-O	-5.50	1.17	1.24
1	C	24	ASN	CA-C	-5.49	1.45	1.52
1	E	118	LEU	C-O	-5.32	1.17	1.23
1	A	122	GLU	C-O	-5.28	1.18	1.23
1	F	2	LEU	N-CA	5.21	1.52	1.46
1	F	166	GLY	N-CA	5.20	1.50	1.45
1	F	164	LYS	C-O	5.18	1.30	1.23
1	D	67	ILE	C-O	-5.17	1.18	1.24
1	A	122	GLU	CA-CB	5.17	1.60	1.53
1	A	124	GLU	CA-CB	5.13	1.60	1.53
1	C	120	GLU	N-CA	-5.11	1.40	1.46
1	F	165	GLU	N-CA	5.11	1.52	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	164	LYS	N-CA-C	-11.08	93.34	109.96
1	F	48	VAL	CB-CA-C	-10.42	94.97	110.81
1	C	48	VAL	CB-CA-C	-10.41	94.99	110.81
1	D	48	VAL	CB-CA-C	-10.31	95.14	110.81
1	B	48	VAL	CB-CA-C	-10.22	95.27	110.81
1	E	48	VAL	CB-CA-C	-10.04	95.54	110.81
1	D	119	LEU	O-C-N	-9.97	111.43	123.30
1	A	48	VAL	CB-CA-C	-9.86	95.82	110.81
1	F	119	LEU	O-C-N	-9.80	110.49	123.23
1	B	70	LEU	CB-CG-CD1	9.69	139.76	110.70
1	F	130	GLU	N-CA-C	9.60	131.25	110.80
1	A	124	GLU	N-CA-C	-8.90	99.49	110.88
1	A	122	GLU	CA-C-O	-8.76	111.69	120.89
1	A	96	SER	N-CA-C	8.38	124.10	113.55
1	E	96	SER	N-CA-C	8.19	123.82	112.93
1	B	53	ARG	CA-CB-CG	-8.18	97.73	114.10
1	B	257	ARG	CG-CD-NE	-7.64	95.18	112.00
1	D	124	GLU	N-CA-C	7.56	120.48	111.33
1	C	132	ASP	N-CA-C	-7.55	98.16	109.86
1	A	129	PRO	N-CA-C	-7.45	97.11	112.47
1	E	105	ASN	CB-CA-C	7.45	121.68	109.46
1	F	105	ASN	CB-CA-C	7.21	122.44	109.61
1	A	1	MET	CG-SD-CE	7.16	116.65	100.90
1	E	277	VAL	CG1-CB-CG2	7.14	126.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	VAL	CG1-CB-CG2	7.11	126.44	110.80
1	D	117	LYS	CA-CB-CG	6.96	128.02	114.10
1	A	126	MET	CB-CA-C	-6.89	107.59	115.79
1	F	275	ASP	N-CA-C	6.82	125.33	110.80
1	C	128	ILE	O-C-N	-6.82	113.33	121.10
1	E	135	SER	N-CA-CB	6.77	121.94	110.49
1	C	105	ASN	CB-CA-C	-6.50	97.37	110.17
1	A	95	ASP	N-CA-CB	-6.42	101.88	111.25
1	A	130	GLU	CB-CA-C	6.41	120.36	109.53
1	D	120	GLU	CA-C-O	-6.40	111.36	120.51
1	F	276	ASN	N-CA-C	6.37	124.37	110.80
1	F	131	MET	N-CA-C	6.18	123.96	110.80
1	A	105	ASN	CB-CA-C	-6.16	98.03	110.17
1	F	127	GLY	N-CA-C	6.15	124.82	113.76
1	B	164	LYS	CA-CB-CG	6.11	126.32	114.10
1	B	105	ASN	CB-CA-C	-6.07	98.22	110.17
1	E	80	LYS	CB-CG-CD	6.03	125.17	111.30
1	F	108	LYS	CB-CG-CD	6.03	125.17	111.30
1	D	105	ASN	CB-CA-C	-5.96	98.43	110.17
1	E	277	VAL	N-CA-CB	-5.95	104.36	112.28
1	F	165	GLU	CA-C-O	-5.81	114.41	119.18
1	F	165	GLU	CB-CA-C	5.74	115.51	109.83
1	E	95	ASP	N-CA-CB	-5.71	102.91	111.25
1	E	130	GLU	N-CA-C	5.70	118.71	110.28
1	A	122	GLU	N-CA-C	-5.67	102.24	111.04
1	C	111	LYS	CG-CD-CE	5.66	124.31	111.30
1	F	120	GLU	CA-C-O	-5.63	112.46	120.51
1	B	270	VAL	CB-CA-C	5.57	117.93	110.42
1	F	40	MET	CG-SD-CE	5.54	113.08	100.90
1	B	132	ASP	N-CA-C	-5.53	100.67	109.96
1	D	184	ALA	N-CA-C	5.47	117.05	111.14
1	D	119	LEU	CA-C-N	5.47	131.99	121.54
1	D	119	LEU	C-N-CA	5.47	131.99	121.54
1	A	94	ASP	CB-CA-C	-5.43	101.72	110.74
1	A	164	LYS	CA-CB-CG	5.35	124.81	114.10
1	D	108	LYS	CB-CG-CD	5.32	123.53	111.30
1	C	236	ILE	N-CA-C	5.31	115.83	108.23
1	E	80	LYS	CG-CD-CE	5.31	123.51	111.30
1	C	111	LYS	CB-CG-CD	5.25	123.39	111.30
1	F	119	LEU	CA-C-N	5.23	131.53	121.54
1	F	119	LEU	C-N-CA	5.23	131.53	121.54
1	C	270	VAL	CB-CA-C	5.22	118.19	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	LYS	CB-CG-CD	5.19	123.23	111.30
1	D	277	VAL	N-CA-CB	-5.17	105.40	112.28
1	D	120	GLU	CA-CB-CG	5.17	124.44	114.10
1	E	270	VAL	CB-CA-C	5.16	118.09	110.77
1	D	287	LYS	CA-C-N	5.13	131.21	121.97
1	D	287	LYS	C-N-CA	5.13	131.21	121.97
1	B	126	MET	N-CA-C	5.13	121.73	110.80
1	E	124	GLU	N-CA-C	5.12	121.70	110.80
1	D	270	VAL	CB-CA-C	5.10	118.01	110.77
1	B	70	LEU	CB-CG-CD2	-5.05	95.55	110.70
1	F	19	ILE	CB-CG1-CD1	-5.03	103.24	113.80
1	F	270	VAL	CB-CA-C	5.03	117.91	110.77
1	B	289	ASP	N-CA-CB	-5.00	101.99	110.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	GLU	Peptide
1	A	276	ASN	Sidechain
1	B	130	GLU	Peptide
1	B	288	VAL	Peptide
1	C	128	ILE	Peptide
1	C	132	ASP	Peptide
1	D	119	LEU	Peptide
1	F	119	LEU	Peptide
1	F	125	SER	Peptide
1	F	165	GLU	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	1919	0	1914	29	0
1	B	1919	0	1914	20	0
1	C	1919	0	1914	38	0
1	D	1919	0	1914	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1919	0	1914	28	0
1	F	1919	0	1914	21	0
2	A	7	0	10	0	0
2	E	7	0	10	1	0
3	A	55	0	0	3	0
3	B	26	0	0	1	0
3	C	30	0	0	2	0
3	D	59	0	0	2	0
3	E	53	0	0	0	0
3	F	27	0	0	1	0
All	All	11778	0	11504	160	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 7.

All (160) 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:1:MET:HE2	1:A:94:ASP:HA	1.43	0.98
1:C:233:GLU:O	1:C:234:GLU:HB2	1.75	0.85
1:C:163:SER:C	1:C:232:MET:HE1	2.04	0.82
1:C:232:MET:CG	1:C:234:GLU:O	2.35	0.74
1:C:164:LYS:N	1:C:232:MET:HE1	2.06	0.71
1:C:232:MET:HG3	1:C:234:GLU:O	1.91	0.70
1:C:93:ASP:HB2	1:C:96:SER:OG	1.92	0.67
1:B:124:GLU:HB2	1:B:126:MET:SD	2.35	0.65
1:C:232:MET:HG2	1:C:234:GLU:O	1.99	0.62
1:A:233:GLU:C	1:A:234:GLU:HG3	2.23	0.62
1:F:22:LEU:HD12	1:F:48:VAL:HG22	1.83	0.60
1:E:22:LEU:HD12	1:E:48:VAL:HG22	1.83	0.60
1:E:56:CYS:HB2	1:E:277:VAL:HG13	1.84	0.60
1:A:24:ASN:HB3	3:A:427:HOH:O	2.03	0.59
1:F:229:GLU:HG2	3:F:325:HOH:O	2.03	0.59
1:A:126:MET:HE3	1:A:126:MET:HA	1.84	0.58
1:A:38:GLN:HG2	1:A:126:MET:HE2	1.85	0.58
1:F:269:MET:HE3	1:F:271:GLU:HB2	1.85	0.58
1:C:22:LEU:HD12	1:C:48:VAL:HG22	1.86	0.58
1:E:163:SER:C	1:E:232:MET:HE3	2.28	0.58
1:E:182:LEU:HD12	1:E:182:LEU:N	2.18	0.58
1:D:56:CYS:HB2	1:D:277:VAL:HG13	1.85	0.57
1:A:163:SER:C	1:A:232:MET:HE3	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:HB3	1:A:55:ASP:OD1	2.05	0.57
1:D:56:CYS:CB	1:D:277:VAL:HG13	2.35	0.57
1:D:48:VAL:HG13	1:D:282:TYR:CE1	2.40	0.57
1:A:1:MET:HE2	1:A:94:ASP:CA	2.26	0.57
1:A:163:SER:C	1:A:232:MET:CE	2.78	0.56
1:B:269:MET:HE3	1:B:271:GLU:HB2	1.87	0.56
1:B:48:VAL:HG13	1:B:282:TYR:CE1	2.40	0.56
1:C:135:SER:OG	1:C:236:ILE:HD11	2.05	0.56
1:C:269:MET:HE3	1:C:271:GLU:HB2	1.87	0.56
1:A:22:LEU:HD12	1:A:48:VAL:HG22	1.87	0.56
1:D:269:MET:HE3	1:D:271:GLU:HB2	1.88	0.56
1:E:56:CYS:CB	1:E:277:VAL:HG13	2.36	0.56
1:E:269:MET:HE3	1:E:271:GLU:HB2	1.88	0.56
1:A:118:LEU:C	1:A:119:LEU:HD12	2.31	0.56
1:E:53:ARG:HB3	1:E:55:ASP:OD1	2.06	0.56
1:C:48:VAL:HG13	1:C:282:TYR:CE1	2.41	0.55
1:D:53:ARG:HG3	3:D:307:HOH:O	2.06	0.55
1:E:24:ASN:OD1	2:E:301:PEG:H41	2.06	0.55
1:C:15:LEU:HD13	1:C:50:MET:CE	2.36	0.55
1:E:163:SER:C	1:E:232:MET:CE	2.80	0.55
1:F:51:LEU:HD23	1:F:279:TYR:CE1	2.42	0.55
1:C:130:GLU:N	1:C:130:GLU:OE1	2.39	0.55
1:F:48:VAL:HG13	1:F:282:TYR:CE1	2.42	0.55
1:F:164:LYS:O	1:F:165:GLU:OE1	2.25	0.54
1:A:48:VAL:HG13	1:A:282:TYR:CE1	2.42	0.54
3:A:413:HOH:O	1:E:122:GLU:HB2	2.08	0.54
1:D:129:PRO:HB2	1:D:131:MET:HE1	1.88	0.54
1:B:51:LEU:HD23	1:B:279:TYR:CE1	2.42	0.54
1:D:129:PRO:HB2	1:D:131:MET:CE	2.38	0.54
1:E:48:VAL:HG13	1:E:282:TYR:CE1	2.43	0.54
1:C:53:ARG:HB3	1:C:55:ASP:OD1	2.08	0.54
1:A:243:ARG:HD3	3:A:421:HOH:O	2.08	0.53
1:D:53:ARG:HB3	1:D:55:ASP:OD1	2.08	0.53
1:E:124:GLU:OE1	1:E:126:MET:O	2.25	0.53
1:F:106:PRO:O	1:F:108:LYS:HD2	2.07	0.53
1:C:51:LEU:HD23	1:C:279:TYR:CE1	2.43	0.53
1:A:269:MET:HE3	1:A:271:GLU:HB2	1.88	0.53
1:C:163:SER:C	1:C:232:MET:CE	2.80	0.53
1:A:15:LEU:HD22	1:A:50:MET:HE3	1.91	0.52
1:B:15:LEU:HD13	1:B:50:MET:CE	2.39	0.51
1:F:31:ASN:ND2	1:F:65:ASN:HD22	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASN:OD1	1:E:122:GLU:OE2	2.28	0.51
1:E:14:ARG:HD2	1:E:253:THR:HB	1.92	0.51
1:C:135:SER:OG	1:C:236:ILE:CD1	2.58	0.51
1:F:15:LEU:HD13	1:F:50:MET:CE	2.41	0.51
1:D:14:ARG:HD2	1:D:253:THR:HB	1.92	0.50
1:B:22:LEU:HD23	1:B:48:VAL:HG22	1.95	0.49
1:A:14:ARG:HD2	1:A:253:THR:HB	1.94	0.49
1:C:40:MET:HG3	1:C:124:GLU:OE2	2.12	0.49
1:B:51:LEU:HD23	1:B:279:TYR:HE1	1.78	0.49
1:C:14:ARG:HD2	1:C:253:THR:HB	1.95	0.49
1:C:19:ILE:HD12	1:C:37:VAL:HG11	1.94	0.49
1:F:14:ARG:HD2	1:F:253:THR:HB	1.94	0.49
1:D:129:PRO:CB	1:D:131:MET:HE1	2.43	0.49
1:B:14:ARG:HD2	1:B:253:THR:HB	1.94	0.48
1:A:78:VAL:O	1:A:81:ILE:HG12	2.13	0.48
1:E:15:LEU:HD22	1:E:50:MET:HE3	1.94	0.48
1:B:78:VAL:O	1:B:81:ILE:HG12	2.14	0.48
1:C:78:VAL:O	1:C:81:ILE:HG12	2.13	0.48
1:C:97:ASP:O	1:C:97:ASP:OD1	2.31	0.48
1:E:78:VAL:O	1:E:81:ILE:HG12	2.14	0.48
1:F:78:VAL:O	1:F:81:ILE:HG12	2.14	0.48
1:F:70:LEU:HD21	1:F:99:VAL:HG11	1.96	0.48
1:D:78:VAL:O	1:D:81:ILE:HG12	2.13	0.48
1:C:161:ALA:CB	1:C:237:THR:HG22	2.44	0.47
1:E:181:PHE:C	1:E:182:LEU:HD12	2.39	0.47
1:E:1:MET:SD	1:E:94:ASP:HA	2.54	0.47
1:D:130:GLU:N	1:D:130:GLU:OE1	2.47	0.47
1:F:90:LEU:C	1:F:90:LEU:HD23	2.40	0.47
1:F:106:PRO:O	1:F:108:LYS:HE2	2.15	0.47
1:A:123:ALA:HB1	1:A:125:SER:OG	2.16	0.46
1:B:19:ILE:HD12	1:B:37:VAL:HG11	1.97	0.46
1:C:24:ASN:ND2	3:C:303:HOH:O	2.48	0.46
1:C:153:VAL:HG22	1:C:154:PHE:CE1	2.51	0.46
1:E:19:ILE:HD12	1:E:37:VAL:HG11	1.97	0.46
1:E:134:ARG:O	1:E:135:SER:OG	2.26	0.46
1:D:136:THR:HG22	3:D:317:HOH:O	2.16	0.45
1:C:70:LEU:HD21	1:C:99:VAL:HG11	1.98	0.45
1:F:153:VAL:HG22	1:F:154:PHE:CE1	2.52	0.45
1:D:131:MET:HE3	1:D:267:PRO:O	2.17	0.45
1:F:118:LEU:N	1:F:118:LEU:HD23	2.32	0.45
1:A:70:LEU:HD21	1:A:99:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:GLU:OE1	1:C:165:GLU:N	2.44	0.45
1:D:182:LEU:HB3	1:D:228:VAL:HG21	1.98	0.45
1:B:162:ILE:HG12	1:B:167:VAL:HG12	1.98	0.45
1:C:15:LEU:HD22	1:C:50:MET:HE3	1.99	0.45
1:E:15:LEU:HD13	1:E:50:MET:CE	2.47	0.44
1:A:15:LEU:HD13	1:A:50:MET:CE	2.47	0.44
1:D:19:ILE:HD12	1:D:37:VAL:HG11	1.98	0.44
1:B:15:LEU:HD22	1:B:50:MET:HE3	1.99	0.44
1:E:131:MET:O	1:E:132:ASP:HB2	2.16	0.44
1:B:158:VAL:HB	1:B:242:LEU:HD21	1.99	0.44
1:C:132:ASP:O	1:C:133:TYR:CG	2.71	0.44
1:B:182:LEU:HB3	1:B:228:VAL:HG21	1.98	0.44
1:D:131:MET:O	1:D:132:ASP:CB	2.65	0.44
1:E:165:GLU:N	1:E:165:GLU:OE1	2.50	0.44
1:C:161:ALA:HB1	1:C:237:THR:HG22	2.00	0.44
1:D:40:MET:HG3	1:D:124:GLU:OE2	2.18	0.44
1:D:56:CYS:SG	1:D:277:VAL:HG13	2.58	0.44
1:F:15:LEU:HD22	1:F:50:MET:HE3	1.99	0.44
1:B:165:GLU:OE1	1:B:165:GLU:N	2.44	0.43
1:F:51:LEU:HD23	1:F:279:TYR:HE1	1.81	0.43
1:E:182:LEU:HB3	1:E:228:VAL:HG21	1.99	0.43
1:A:1:MET:CE	1:A:94:ASP:HA	2.29	0.43
1:A:130:GLU:OE2	1:A:130:GLU:HA	2.19	0.43
1:B:161:ALA:CB	1:B:237:THR:HG22	2.49	0.43
1:C:51:LEU:HD23	1:C:279:TYR:HE1	1.81	0.43
1:C:158:VAL:HB	1:C:242:LEU:HD21	2.01	0.43
1:C:276:ASN:OD1	1:C:276:ASN:N	2.50	0.43
1:F:2:LEU:C	1:F:2:LEU:HD23	2.44	0.43
1:C:2:LEU:C	1:C:2:LEU:HD23	2.44	0.42
1:F:182:LEU:HB3	1:F:228:VAL:HG21	2.01	0.42
1:E:182:LEU:N	1:E:182:LEU:CD1	2.82	0.42
1:C:128:ILE:HG22	1:C:129:PRO:HD2	2.01	0.42
1:F:230:VAL:O	1:F:231:THR:HG23	2.19	0.42
1:D:165:GLU:OE1	1:D:165:GLU:N	2.44	0.42
1:E:158:VAL:HB	1:E:242:LEU:HD21	2.01	0.42
1:C:120:GLU:HG3	3:C:327:HOH:O	2.18	0.42
1:A:28:PHE:CE1	1:A:70:LEU:HD12	2.55	0.42
1:E:230:VAL:O	1:E:231:THR:HG23	2.19	0.42
1:A:230:VAL:O	1:A:231:THR:HG23	2.19	0.41
1:D:158:VAL:HB	1:D:242:LEU:HD21	2.02	0.41
1:D:70:LEU:HD21	1:D:99:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LEU:HD23	1:B:2:LEU:C	2.45	0.41
1:D:131:MET:HE2	1:D:133:TYR:OH	2.21	0.41
1:C:15:LEU:HD13	1:C:50:MET:HE2	2.02	0.41
1:D:22:LEU:CD2	1:D:48:VAL:HG22	2.50	0.41
1:C:230:VAL:O	1:C:231:THR:HG23	2.20	0.41
1:A:119:LEU:N	1:A:119:LEU:CD1	2.84	0.41
1:D:22:LEU:HD23	1:D:48:VAL:HG22	2.03	0.41
1:B:22:LEU:CD2	1:B:48:VAL:HG22	2.51	0.41
1:B:149:ARG:HD2	3:B:324:HOH:O	2.21	0.41
1:A:19:ILE:HD12	1:A:37:VAL:HG11	2.03	0.40
1:E:70:LEU:HD21	1:E:99:VAL:HG11	2.03	0.40
1:B:232:MET:HG2	1:B:234:GLU:H	1.86	0.40
1:A:119:LEU:HD12	1:A:119:LEU:N	2.36	0.40
1:A:182:LEU:HB3	1:A:228:VAL:HG21	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	244/292 (84%)	229 (94%)	13 (5%)	2 (1%)	16	29
1	B	244/292 (84%)	230 (94%)	13 (5%)	1 (0%)	30	47
1	C	244/292 (84%)	228 (93%)	12 (5%)	4 (2%)	7	13
1	D	244/292 (84%)	228 (93%)	12 (5%)	4 (2%)	7	13
1	E	244/292 (84%)	227 (93%)	14 (6%)	3 (1%)	10	19
1	F	244/292 (84%)	225 (92%)	15 (6%)	4 (2%)	7	13
All	All	1464/1752 (84%)	1367 (93%)	79 (5%)	18 (1%)	10	19

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	135	SER
1	C	129	PRO
1	C	234	GLU
1	F	130	GLU
1	C	128	ILE
1	F	131	MET
1	A	129	PRO
1	D	288	VAL
1	E	126	MET
1	F	84	SER
1	A	84	SER
1	D	84	SER
1	D	125	SER
1	E	84	SER
1	B	84	SER
1	C	84	SER
1	F	128	ILE
1	D	132	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/251 (86%)	183 (85%)	33 (15%)	3	3
1	B	216/251 (86%)	184 (85%)	32 (15%)	3	4
1	C	216/251 (86%)	180 (83%)	36 (17%)	2	2
1	D	216/251 (86%)	181 (84%)	35 (16%)	2	3
1	E	216/251 (86%)	181 (84%)	35 (16%)	2	3
1	F	216/251 (86%)	178 (82%)	38 (18%)	2	2
All	All	1296/1506 (86%)	1087 (84%)	209 (16%)	2	3

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL

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Mol	Chain	Res	Type
1	A	10	SER
1	A	19	ILE
1	A	22	LEU
1	A	24	ASN
1	A	48	VAL
1	A	50	MET
1	A	53	ARG
1	A	80	LYS
1	A	81	ILE
1	A	94	ASP
1	A	97	ASP
1	A	98	VAL
1	A	100	THR
1	A	103	SER
1	A	107	GLU
1	A	111	LYS
1	A	116	LEU
1	A	118	LEU
1	A	122	GLU
1	A	131	MET
1	A	136	THR
1	A	137	VAL
1	A	153	VAL
1	A	162	ILE
1	A	164	LYS
1	A	165	GLU
1	A	170	SER
1	A	232	MET
1	A	234	GLU
1	A	270	VAL
1	A	281	ARG
1	A	287	LYS
1	D	1	MET
1	D	6	VAL
1	D	10	SER
1	D	19	ILE
1	D	24	ASN
1	D	48	VAL
1	D	50	MET
1	D	53	ARG
1	D	59	LYS
1	D	80	LYS

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Mol	Chain	Res	Type
1	D	81	ILE
1	D	97	ASP
1	D	98	VAL
1	D	100	THR
1	D	103	SER
1	D	104	GLU
1	D	111	LYS
1	D	116	LEU
1	D	117	LYS
1	D	120	GLU
1	D	136	THR
1	D	137	VAL
1	D	153	VAL
1	D	162	ILE
1	D	163	SER
1	D	164	LYS
1	D	170	SER
1	D	231	THR
1	D	232	MET
1	D	233	GLU
1	D	250	LYS
1	D	266	SER
1	D	270	VAL
1	D	277	VAL
1	D	281	ARG
1	E	1	MET
1	E	10	SER
1	E	19	ILE
1	E	22	LEU
1	E	24	ASN
1	E	48	VAL
1	E	50	MET
1	E	53	ARG
1	E	80	LYS
1	E	81	ILE
1	E	94	ASP
1	E	97	ASP
1	E	98	VAL
1	E	100	THR
1	E	103	SER
1	E	104	GLU
1	E	116	LEU

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Mol	Chain	Res	Type
1	E	117	LYS
1	E	118	LEU
1	E	125	SER
1	E	126	MET
1	E	132	ASP
1	E	134	ARG
1	E	136	THR
1	E	137	VAL
1	E	164	LYS
1	E	165	GLU
1	E	170	SER
1	E	232	MET
1	E	234	GLU
1	E	264	LYS
1	E	265	ASP
1	E	270	VAL
1	E	277	VAL
1	E	281	ARG
1	B	6	VAL
1	B	10	SER
1	B	19	ILE
1	B	24	ASN
1	B	48	VAL
1	B	50	MET
1	B	64	ARG
1	B	70	LEU
1	B	80	LYS
1	B	81	ILE
1	B	100	THR
1	B	103	SER
1	B	104	GLU
1	B	107	GLU
1	B	116	LEU
1	B	117	LYS
1	B	118	LEU
1	B	125	SER
1	B	132	ASP
1	B	134	ARG
1	B	136	THR
1	B	137	VAL
1	B	162	ILE
1	B	164	LYS

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Mol	Chain	Res	Type
1	B	167	VAL
1	B	170	SER
1	B	232	MET
1	B	233	GLU
1	B	234	GLU
1	B	264	LYS
1	B	270	VAL
1	B	281	ARG
1	C	6	VAL
1	C	10	SER
1	C	19	ILE
1	C	22	LEU
1	C	47	LEU
1	C	48	VAL
1	C	50	MET
1	C	53	ARG
1	C	64	ARG
1	C	80	LYS
1	C	81	ILE
1	C	100	THR
1	C	103	SER
1	C	104	GLU
1	C	105	ASN
1	C	107	GLU
1	C	111	LYS
1	C	116	LEU
1	C	117	LYS
1	C	126	MET
1	C	130	GLU
1	C	131	MET
1	C	134	ARG
1	C	136	THR
1	C	137	VAL
1	C	162	ILE
1	C	170	SER
1	C	183	GLN
1	C	232	MET
1	C	236	ILE
1	C	264	LYS
1	C	270	VAL
1	C	276	ASN
1	C	281	ARG

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Mol	Chain	Res	Type
1	C	287	LYS
1	C	289	ASP
1	F	6	VAL
1	F	10	SER
1	F	19	ILE
1	F	22	LEU
1	F	24	ASN
1	F	48	VAL
1	F	50	MET
1	F	53	ARG
1	F	55	ASP
1	F	64	ARG
1	F	80	LYS
1	F	81	ILE
1	F	97	ASP
1	F	98	VAL
1	F	100	THR
1	F	103	SER
1	F	107	GLU
1	F	108	LYS
1	F	116	LEU
1	F	118	LEU
1	F	125	SER
1	F	128	ILE
1	F	130	GLU
1	F	131	MET
1	F	132	ASP
1	F	136	THR
1	F	137	VAL
1	F	148	VAL
1	F	162	ILE
1	F	165	GLU
1	F	170	SER
1	F	232	MET
1	F	233	GLU
1	F	250	LYS
1	F	264	LYS
1	F	266	SER
1	F	270	VAL
1	F	281	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	D	38	GLN
1	D	61	GLN
1	D	92	HIS
1	D	115	GLN
1	D	183	GLN
1	E	31	ASN
1	E	38	GLN
1	E	92	HIS
1	B	38	GLN
1	B	61	GLN
1	C	31	ASN
1	C	38	GLN
1	C	49	HIS
1	C	92	HIS
1	C	105	ASN
1	C	115	GLN
1	F	38	GLN
1	F	44	HIS
1	F	65	ASN
1	F	92	HIS
1	F	276	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	PEG	E	301	-	6,6,6	0.83	0	5,5,5	0.94	0
2	PEG	A	301	-	6,6,6	0.56	0	5,5,5	0.37	0

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	PEG	E	301	-	-	3/4/4/4	-
2	PEG	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PEG	O1-C1-C2-O2
2	E	301	PEG	O1-C1-C2-O2
2	A	301	PEG	O2-C3-C4-O4
2	E	301	PEG	O2-C3-C4-O4
2	E	301	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	PEG	1	0

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

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	248/292 (84%)	-0.02	8 (3%)	50	48	50, 75, 127, 177	0
1	B	248/292 (84%)	0.39	12 (4%)	35	35	59, 91, 140, 171	0
1	C	248/292 (84%)	0.48	17 (6%)	23	22	63, 92, 152, 187	0
1	D	248/292 (84%)	0.25	9 (3%)	46	44	51, 83, 139, 182	0
1	E	248/292 (84%)	0.16	10 (4%)	42	40	55, 82, 138, 160	0
1	F	248/292 (84%)	0.49	17 (6%)	23	22	64, 99, 157, 195	0
All	All	1488/1752 (84%)	0.29	73 (4%)	35	35	50, 88, 145, 195	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	VAL	7.1
1	D	126	MET	5.1
1	D	1	MET	4.7
1	C	185	ALA	4.6
1	C	129	PRO	4.4
1	D	185	ALA	4.1
1	F	126	MET	4.0
1	C	123	ALA	4.0
1	B	126	MET	4.0
1	B	185	ALA	4.0
1	C	169	PHE	4.0
1	F	131	MET	4.0
1	C	236	ILE	3.8
1	F	1	MET	3.7
1	E	64	ARG	3.7
1	C	288	VAL	3.6
1	B	174	ASP	3.4
1	A	288	VAL	3.4
1	F	129	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	126	MET	3.3
1	F	231	THR	3.2
1	C	1	MET	3.1
1	E	131	MET	3.0
1	B	1	MET	3.0
1	C	235	PRO	3.0
1	C	131	MET	3.0
1	B	262	PHE	3.0
1	F	288	VAL	3.0
1	C	96	SER	2.9
1	B	64	ARG	2.9
1	D	127	GLY	2.9
1	C	231	THR	2.9
1	C	227	GLY	2.9
1	F	227	GLY	2.8
1	E	288	VAL	2.8
1	A	164	LYS	2.7
1	F	128	ILE	2.7
1	B	227	GLY	2.7
1	F	123	ALA	2.6
1	E	94	ASP	2.6
1	B	94	ASP	2.6
1	C	250	LYS	2.6
1	F	28	PHE	2.6
1	A	231	THR	2.5
1	F	264	LYS	2.5
1	E	97	ASP	2.5
1	E	1	MET	2.5
1	A	64	ARG	2.4
1	F	63	GLY	2.4
1	B	231	THR	2.4
1	A	175	VAL	2.4
1	F	267	PRO	2.3
1	D	63	GLY	2.3
1	E	185	ALA	2.3
1	C	134	ARG	2.3
1	A	1	MET	2.3
1	F	127	GLY	2.3
1	E	167	VAL	2.3
1	A	123	ALA	2.2
1	C	237	THR	2.2
1	B	250	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	235	PRO	2.1
1	F	94	ASP	2.1
1	F	160	ILE	2.1
1	D	250	LYS	2.1
1	B	164	LYS	2.1
1	E	166	GLY	2.1
1	A	169	PHE	2.1
1	D	125	SER	2.1
1	E	123	ALA	2.0
1	B	63	GLY	2.0
1	C	128	ILE	2.0
1	D	94	ASP	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
2	PEG	A	301	7/7	0.94	0.16	93,113,124,140	0
2	PEG	E	301	7/7	0.94	0.12	88,99,105,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.