



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:38 AM UTC

PDB ID : 3EBJ / pdb_00003ebj
Title : Crystal structure of an avian influenza virus protein
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Deposited on : 2008-08-27
Resolution : 2.20 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

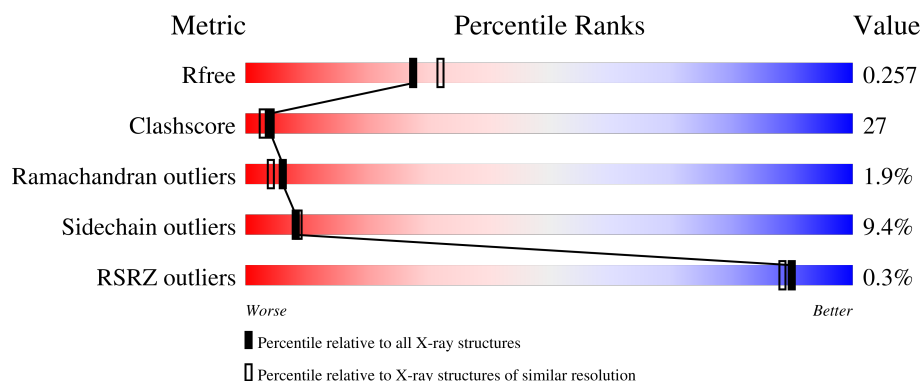
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	259	36% 27% 5% 32%
1	B	259	35% 27% • • 32%
1	C	259	37% 25% • • 32%
1	D	259	31% 30% 7% 32%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5925 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			
1	B	175	Total	C	N	O	S	0	0	0
			1458	923	250	274	11			
1	C	176	Total	C	N	O	S	0	0	0
			1456	920	252	273	11			
1	D	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	LEU	-	expression tag	UNP Q9Q0U9
A	-1	GLY	-	expression tag	UNP Q9Q0U9
A	0	SER	-	expression tag	UNP Q9Q0U9
A	201	ILE	VAL	engineered mutation	UNP Q9Q0U9
B	-2	LEU	-	expression tag	UNP Q9Q0U9
B	-1	GLY	-	expression tag	UNP Q9Q0U9
B	0	SER	-	expression tag	UNP Q9Q0U9
B	201	ILE	VAL	engineered mutation	UNP Q9Q0U9
C	-2	LEU	-	expression tag	UNP Q9Q0U9
C	-1	GLY	-	expression tag	UNP Q9Q0U9
C	0	SER	-	expression tag	UNP Q9Q0U9
C	201	ILE	VAL	engineered mutation	UNP Q9Q0U9
D	-2	LEU	-	expression tag	UNP Q9Q0U9
D	-1	GLY	-	expression tag	UNP Q9Q0U9
D	0	SER	-	expression tag	UNP Q9Q0U9
D	201	ILE	VAL	engineered mutation	UNP Q9Q0U9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0

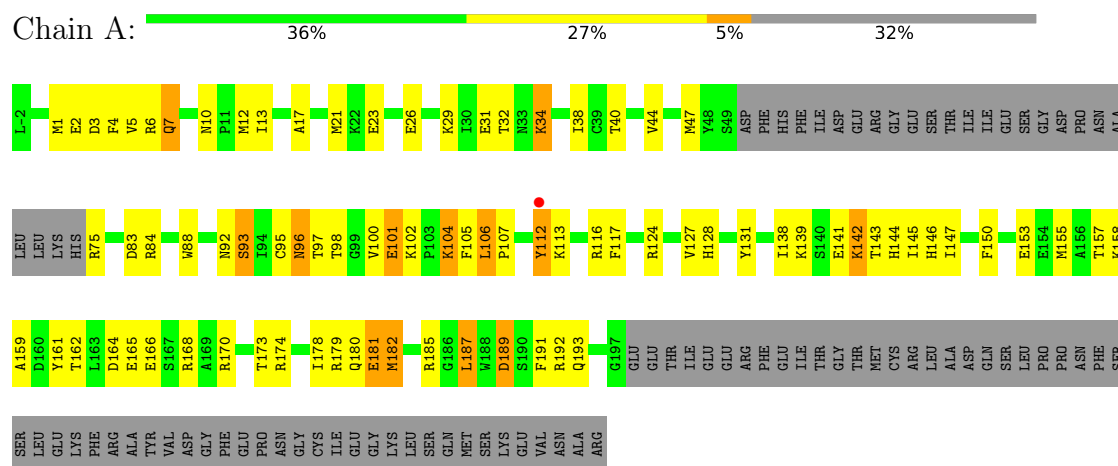
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total 40	O 40	0	0
3	B	28	Total 28	O 28	0	0
3	C	22	Total 22	O 22	0	0
3	D	25	Total 25	O 25	0	0

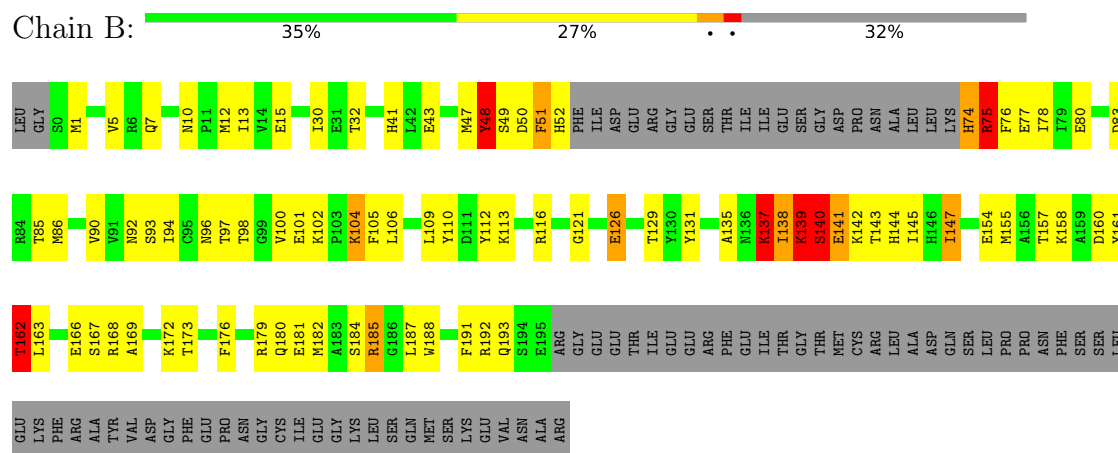
3 Residue-property plots

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.

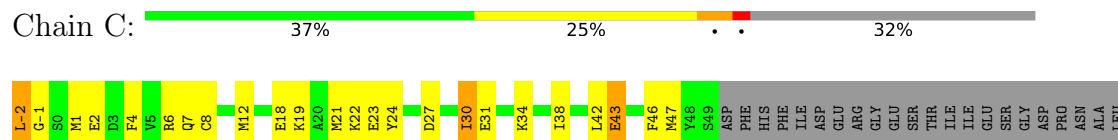
• Molecule 1: Polymerase acidic protein

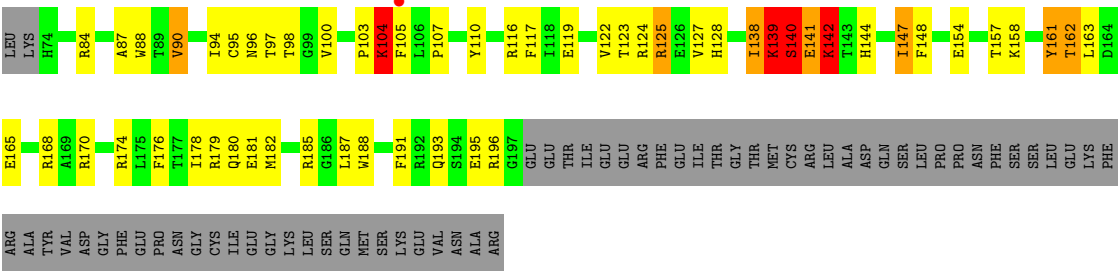


• Molecule 1: Polymerase acidic protein

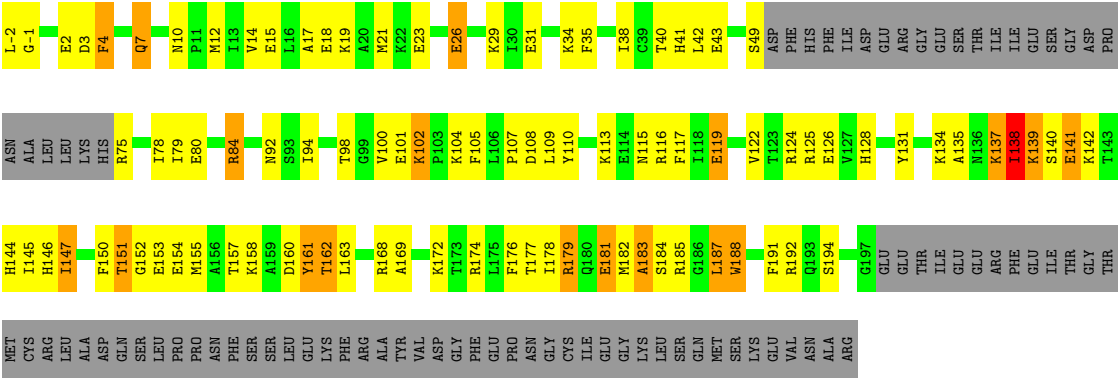
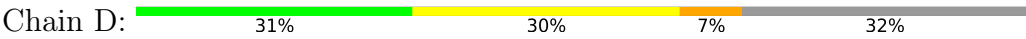


• Molecule 1: Polymerase acidic protein





● Molecule 1: Polymerase acidic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.05Å 59.83Å 67.17Å 96.55° 96.82° 109.51°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 80.4 (50.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.252 0.234 , 0.257	Depositor DCC
R_{free} test set	1665 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5925	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% 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: MG

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	1.07	12/1474 (0.8%)	1.14	10/1977 (0.5%)
1	B	1.56	42/1489 (2.8%)	1.25	15/1999 (0.8%)
1	C	1.34	25/1485 (1.7%)	1.19	15/1992 (0.8%)
1	D	0.53	0/1474	0.99	7/1977 (0.4%)
All	All	1.19	79/5922 (1.3%)	1.15	47/7945 (0.6%)

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	B	0	1
1	D	0	1
All	All	0	2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	ILE	C-O	-16.60	1.05	1.24
1	B	160	ASP	C-O	-15.79	1.05	1.24
1	A	105	PHE	C-O	-14.97	1.04	1.24
1	B	49	SER	C-O	-14.07	1.07	1.23
1	C	142	LYS	C-O	-13.21	1.07	1.24
1	C	103	PRO	C-O	-12.30	1.07	1.24
1	A	104	LYS	C-O	-12.22	1.07	1.24
1	B	161	TYR	C-O	-11.26	1.10	1.23
1	B	49	SER	CA-CB	-11.18	1.38	1.53
1	B	161	TYR	N-CA	-10.91	1.32	1.45
1	B	162	THR	C-O	-10.83	1.10	1.23
1	C	105	PHE	C-O	-10.52	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	ILE	CB-CG2	-10.49	1.18	1.52
1	B	138	ILE	CB-CG2	-10.40	1.18	1.52
1	A	105	PHE	CD2-CE2	-10.31	1.07	1.38
1	A	106	LEU	C-O	-10.24	1.10	1.24
1	B	51	PHE	CE2-CZ	-9.99	1.08	1.38
1	B	160	ASP	CA-C	-9.51	1.40	1.53
1	B	162	THR	C-N	-9.06	1.20	1.33
1	C	103	PRO	CB-CG	-9.06	1.04	1.49
1	A	105	PHE	CE2-CZ	-8.90	1.11	1.38
1	B	141	GLU	C-O	-8.76	1.12	1.24
1	B	138	ILE	CG1-CD1	-8.72	1.17	1.51
1	A	105	PHE	CD1-CE1	-8.66	1.12	1.38
1	B	161	TYR	CA-C	-8.61	1.41	1.52
1	A	104	LYS	CA-CB	-8.17	1.41	1.53
1	C	141	GLU	N-CA	-8.14	1.36	1.46
1	C	141	GLU	C-O	-8.11	1.09	1.23
1	B	162	THR	CB-CG2	-7.99	1.26	1.52
1	C	142	LYS	C-N	-7.86	1.22	1.33
1	C	140	SER	C-O	-7.80	1.07	1.23
1	B	139	LYS	CA-C	-7.63	1.42	1.52
1	C	142	LYS	CA-CB	-7.56	1.42	1.54
1	C	139	LYS	C-O	-7.53	1.14	1.24
1	C	104	LYS	C-O	-7.27	1.14	1.24
1	C	140	SER	C-N	-7.25	1.23	1.33
1	C	141	GLU	CA-C	-7.19	1.40	1.53
1	B	140	SER	CA-C	-7.14	1.43	1.52
1	A	104	LYS	CG-CD	-7.10	1.31	1.52
1	C	104	LYS	N-CA	-6.87	1.37	1.46
1	B	160	ASP	CG-OD1	-6.67	1.12	1.25
1	B	51	PHE	CD2-CE2	-6.66	1.18	1.38
1	B	51	PHE	CE1-CZ	-6.56	1.19	1.38
1	C	138	ILE	N-CA	-6.56	1.38	1.46
1	A	104	LYS	CB-CG	-6.55	1.32	1.52
1	A	105	PHE	CE1-CZ	-6.43	1.19	1.38
1	B	138	ILE	CA-C	-6.38	1.43	1.52
1	B	50	ASP	CG-OD2	-6.35	1.13	1.25
1	B	49	SER	N-CA	-6.32	1.38	1.46
1	B	162	THR	CA-CB	-6.27	1.45	1.54
1	B	160	ASP	CG-OD2	-6.14	1.13	1.25
1	C	105	PHE	CA-C	-6.12	1.45	1.52
1	C	103	PRO	C-N	-6.05	1.25	1.33
1	A	104	LYS	N-CA	-6.01	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	PHE	CG-CD1	-6.01	1.26	1.38
1	B	49	SER	CB-OG	-5.99	1.30	1.42
1	B	161	TYR	CZ-OH	-5.94	1.25	1.38
1	B	51	PHE	C-O	-5.91	1.16	1.23
1	B	137	LYS	C-N	-5.90	1.27	1.34
1	C	103	PRO	CA-CB	-5.87	1.45	1.53
1	C	142	LYS	CB-CG	-5.76	1.35	1.52
1	B	50	ASP	CG-OD1	-5.75	1.14	1.25
1	B	138	ILE	CA-CB	-5.75	1.46	1.54
1	B	162	THR	N-CA	5.74	1.53	1.45
1	B	161	TYR	C-N	-5.74	1.25	1.33
1	B	139	LYS	CG-CD	-5.65	1.35	1.52
1	B	137	LYS	C-O	-5.65	1.16	1.24
1	C	105	PHE	CE2-CZ	-5.63	1.21	1.38
1	B	138	ILE	N-CA	-5.60	1.38	1.46
1	A	106	LEU	CA-CB	-5.59	1.43	1.53
1	B	161	TYR	CE2-CZ	-5.51	1.25	1.38
1	C	103	PRO	CG-CD	-5.51	1.32	1.50
1	B	48	TYR	C-N	-5.46	1.24	1.33
1	B	140	SER	CA-CB	-5.43	1.44	1.53
1	C	141	GLU	C-N	-5.38	1.25	1.33
1	C	103	PRO	N-CA	-5.30	1.40	1.47
1	B	139	LYS	CA-CB	-5.18	1.44	1.53
1	B	137	LYS	CD-CE	5.18	1.68	1.52
1	B	141	GLU	CA-C	-5.12	1.46	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	THR	CA-C-O	12.43	132.27	118.97
1	A	97	THR	N-CA-C	-12.26	98.46	113.41
1	B	140	SER	N-CA-C	10.54	133.24	110.80
1	A	106	LEU	N-CA-C	8.71	120.89	109.83
1	C	138	ILE	N-CA-C	8.65	122.75	112.80
1	A	106	LEU	CA-C-O	-8.34	111.24	120.25
1	B	161	TYR	O-C-N	-8.06	114.04	123.06
1	B	51	PHE	N-CA-C	7.38	121.17	109.50
1	A	105	PHE	N-CA-C	-7.12	97.80	109.40
1	D	4	PHE	N-CA-C	-7.11	100.68	111.56
1	B	76	PHE	N-CA-C	7.08	121.37	109.76
1	B	161	TYR	CA-C-N	-7.07	110.51	122.11
1	B	161	TYR	C-N-CA	-7.07	110.51	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	PHE	O-C-N	-6.87	114.30	123.23
1	C	125	ARG	N-CA-C	6.69	114.26	108.78
1	B	75	ARG	N-CA-C	6.49	124.62	110.80
1	B	49	SER	N-CA-C	6.39	119.64	107.75
1	C	138	ILE	CG1-CB-CG2	-6.37	91.58	110.70
1	D	183	ALA	N-CA-C	-6.18	103.86	112.45
1	A	192	ARG	N-CA-C	6.07	118.69	111.71
1	B	30	ILE	N-CA-C	-6.05	105.79	111.48
1	A	113	LYS	N-CA-C	-6.03	103.47	111.24
1	D	141	GLU	N-CA-C	-6.01	105.79	113.01
1	B	161	TYR	N-CA-C	-5.87	100.99	110.32
1	D	102	LYS	N-CA-C	-5.84	102.71	110.07
1	C	139	LYS	CB-CG-CD	5.79	124.61	111.30
1	B	32	THR	N-CA-C	5.67	118.39	111.82
1	D	35	PHE	N-CA-C	-5.59	105.28	111.71
1	A	181	GLU	N-CA-C	-5.46	105.88	112.54
1	D	188	TRP	N-CA-C	5.42	118.68	111.75
1	C	142	LYS	CA-C-N	-5.40	115.01	122.30
1	C	142	LYS	C-N-CA	-5.40	115.01	122.30
1	C	140	SER	N-CA-C	-5.36	96.00	111.00
1	A	182	MET	N-CA-C	-5.33	105.51	112.23
1	C	-1	GLY	N-CA-C	-5.33	104.42	112.41
1	C	142	LYS	CD-CE-NZ	5.28	128.80	111.90
1	B	140	SER	CA-CB-OG	-5.20	100.70	111.10
1	C	138	ILE	O-C-N	-5.19	116.36	122.07
1	C	125	ARG	CB-CA-C	-5.18	109.62	117.07
1	C	105	PHE	CA-C-O	-5.13	115.11	121.06
1	A	5	VAL	N-CA-C	5.12	115.73	110.36
1	C	161	TYR	N-CA-C	5.12	119.21	112.92
1	B	48	TYR	O-C-N	-5.05	116.77	122.12
1	C	103	PRO	CA-N-CD	-5.01	104.98	112.00
1	C	8	CYS	N-CA-C	5.01	117.51	111.40
1	D	169	ALA	N-CA-C	-5.01	106.01	111.82
1	B	137	LYS	CG-CD-CE	5.00	122.80	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	48	TYR	Mainchain
1	D	161	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	1446	0	1422	70	0
1	B	1458	0	1419	70	0
1	C	1456	0	1429	84	0
1	D	1446	0	1422	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	40	0	0	3	0
3	B	28	0	0	0	0
3	C	22	0	0	5	0
3	D	25	0	0	3	0
All	All	5925	0	5692	316	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 27.

All (316) 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:C:139:LYS:CG	1:C:140:SER:HA	1.41	1.49
1:C:139:LYS:HG2	1:C:140:SER:CA	1.59	1.30
1:C:139:LYS:CG	1:C:140:SER:CA	2.12	1.21
1:C:139:LYS:CB	1:C:140:SER:HA	1.75	1.16
1:C:104:LYS:NZ	1:C:139:LYS:HB2	1.66	1.08
1:C:104:LYS:HZ3	1:C:139:LYS:HB2	1.18	1.07
1:C:139:LYS:CD	1:C:140:SER:HA	1.86	1.05
1:D:84:ARG:HH11	1:D:84:ARG:HB3	1.19	1.05
1:C:27:ASP:HB3	1:C:30:ILE:HD11	1.38	1.03
1:D:101:GLU:OE2	1:D:142:LYS:HE3	1.64	0.98
1:B:52:HIS:HA	1:B:74:HIS:N	1.79	0.97
1:C:139:LYS:CB	1:C:140:SER:CA	2.38	0.95
1:C:84:ARG:HH21	1:C:88:TRP:HE1	1.07	0.95
1:D:147:ILE:HD11	1:D:155:MET:HB3	1.50	0.91
1:B:48:TYR:OH	1:B:162:THR:CG2	2.20	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HB3	1:C:140:SER:HA	1.55	0.89
1:B:138:ILE:O	1:B:139:LYS:HB2	1.72	0.89
1:C:138:ILE:O	1:C:139:LYS:HB3	1.74	0.86
1:C:116:ARG:HD2	1:C:144:HIS:HB2	1.58	0.85
1:C:139:LYS:HG2	1:C:140:SER:N	1.82	0.85
1:D:84:ARG:HB3	1:D:84:ARG:NH1	1.91	0.85
1:A:116:ARG:HD2	1:A:144:HIS:HB2	1.60	0.83
1:C:139:LYS:HB3	1:C:140:SER:CA	2.09	0.82
1:B:92:ASN:HD21	1:B:102:LYS:NZ	1.78	0.80
1:B:48:TYR:OH	1:B:162:THR:HG21	1.81	0.78
1:C:138:ILE:O	1:C:139:LYS:CB	2.28	0.78
1:A:147:ILE:HB	3:A:1031:HOH:O	1.84	0.78
1:C:139:LYS:HD3	1:C:140:SER:HA	1.65	0.77
1:D:182:MET:HE1	1:D:191:PHE:CD2	2.20	0.76
1:C:139:LYS:HG2	1:C:140:SER:C	2.10	0.76
1:B:93:SER:O	1:B:97:THR:HG22	1.85	0.75
1:B:98:THR:HG22	1:B:100:VAL:HG23	1.67	0.75
1:C:27:ASP:CB	1:C:30:ILE:HD11	2.16	0.75
1:D:147:ILE:CD1	1:D:155:MET:HB3	2.16	0.75
1:B:138:ILE:O	1:B:139:LYS:CB	2.30	0.72
1:A:144:HIS:CE1	1:A:157:THR:HB	2.25	0.71
1:D:41:HIS:CE1	3:D:1001:HOH:O	2.43	0.71
1:B:104:LYS:HD3	1:B:104:LYS:N	2.05	0.71
1:A:174:ARG:O	1:A:178:ILE:HG13	1.91	0.71
1:D:182:MET:HE2	1:D:188:TRP:HE3	1.56	0.70
1:D:182:MET:HB2	1:D:188:TRP:HB2	1.73	0.70
1:C:104:LYS:HZ2	1:C:139:LYS:HB2	1.56	0.69
1:C:96:ASN:HD22	1:C:97:THR:HG23	1.58	0.69
1:B:74:HIS:N	1:B:74:HIS:CD2	2.58	0.69
1:A:164:ASP:OD2	1:A:166:GLU:HG2	1.93	0.68
1:D:138:ILE:H	1:D:138:ILE:HD13	1.58	0.68
1:A:185:ARG:HB2	1:A:187:LEU:HD22	1.74	0.68
1:D:134:LYS:HG3	1:D:138:ILE:HD11	1.75	0.68
1:A:96:ASN:H	1:A:96:ASN:HD22	1.41	0.68
1:D:178:ILE:O	1:D:182:MET:HG3	1.93	0.67
1:C:4:PHE:HE1	1:C:181:GLU:HG3	1.59	0.67
1:C:124:ARG:NH2	1:C:195:GLU:HG3	2.10	0.67
1:D:137:LYS:HZ3	1:D:138:ILE:HG23	1.60	0.67
1:A:83:ASP:OD2	1:B:85:THR:HB	1.94	0.67
1:D:141:GLU:CD	1:D:141:GLU:H	2.03	0.67
1:C:139:LYS:HE3	1:C:140:SER:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:HIS:CG	1:A:155:MET:HE1	2.31	0.66
1:C:125:ARG:HD2	3:C:1021:HOH:O	1.94	0.66
1:C:124:ARG:HD2	1:C:191:PHE:CE2	2.30	0.66
1:D:119:GLU:OE1	3:D:1003:HOH:O	2.13	0.65
1:B:154:GLU:OE1	1:B:168:ARG:HD2	1.96	0.65
1:C:27:ASP:HB3	1:C:30:ILE:CD1	2.21	0.65
1:B:192:ARG:NH2	1:B:193:GLN:HE21	1.94	0.65
1:D:154:GLU:OE1	1:D:168:ARG:NH1	2.30	0.64
1:A:96:ASN:H	1:A:96:ASN:ND2	1.95	0.64
1:B:192:ARG:HH21	1:B:193:GLN:HE21	1.44	0.64
1:A:157:THR:HG22	1:A:158:LYS:HG3	1.80	0.64
1:B:98:THR:CG2	1:B:100:VAL:HG23	2.28	0.63
1:D:137:LYS:NZ	1:D:138:ILE:HG23	2.14	0.63
1:B:147:ILE:HD13	1:B:147:ILE:H	1.64	0.62
1:D:158:LYS:HE2	1:D:158:LYS:HA	1.80	0.62
1:C:-2:LEU:N	1:C:-2:LEU:HD12	2.15	0.62
1:C:84:ARG:HH21	1:C:88:TRP:NE1	1.90	0.62
1:C:21:MET:HE3	1:C:34:LYS:HG2	1.82	0.61
1:D:92:ASN:HD21	1:D:102:LYS:NZ	1.97	0.61
1:C:84:ARG:NH2	1:C:88:TRP:HE1	1.88	0.61
1:A:92:ASN:ND2	1:A:102:LYS:NZ	2.49	0.61
1:D:179:ARG:HG2	1:D:188:TRP:CZ3	2.36	0.61
1:D:31:GLU:HB3	1:D:34:LYS:HG2	1.82	0.60
1:C:181:GLU:O	1:C:185:ARG:HG3	2.01	0.60
1:A:98:THR:OG1	1:A:100:VAL:HG23	2.00	0.60
1:D:98:THR:HG22	1:D:100:VAL:HG13	1.84	0.60
1:B:78:ILE:HA	1:B:109:LEU:HD23	1.83	0.59
1:A:3:ASP:O	1:A:7:GLN:HG2	2.02	0.59
1:D:23:GLU:OE1	1:D:84:ARG:HG2	2.01	0.59
1:C:4:PHE:HE1	1:C:181:GLU:CG	2.15	0.59
1:C:43:GLU:O	1:C:47:MET:HG3	2.03	0.59
1:D:98:THR:HG21	1:D:110:TYR:OH	2.03	0.59
1:A:1:MET:HE1	1:A:182:MET:HE2	1.85	0.59
1:D:12:MET:O	1:D:15:GLU:HB2	2.02	0.58
1:A:4:PHE:HE1	1:A:181:GLU:HG3	1.68	0.58
1:B:157:THR:HG22	1:B:158:LYS:HG3	1.85	0.58
1:A:92:ASN:ND2	1:A:102:LYS:HZ2	2.02	0.58
1:D:116:ARG:HD2	1:D:144:HIS:HB2	1.85	0.58
1:B:126:GLU:OE2	1:B:129:THR:HB	2.03	0.58
1:C:30:ILE:HD13	1:C:30:ILE:N	2.19	0.58
1:C:144:HIS:CE1	1:C:157:THR:HB	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:CD	1:C:140:SER:CA	2.64	0.57
1:B:92:ASN:HD21	1:B:102:LYS:HZ1	1.53	0.57
1:C:139:LYS:HD3	1:C:140:SER:CA	2.31	0.57
1:A:83:ASP:OD1	1:B:83:ASP:HB3	2.05	0.57
1:B:166:GLU:O	1:B:169:ALA:HB3	2.05	0.57
1:D:94:ILE:O	1:D:98:THR:HB	2.04	0.57
1:C:139:LYS:HB3	1:C:140:SER:CB	2.34	0.56
1:D:150:PHE:HB3	1:D:179:ARG:HG3	1.88	0.56
1:B:144:HIS:CE1	1:B:157:THR:HB	2.40	0.56
1:A:131:TYR:HD1	3:A:1031:HOH:O	1.88	0.56
1:A:189:ASP:O	1:A:193:GLN:HG2	2.06	0.56
1:B:116:ARG:HD2	1:B:144:HIS:HB2	1.87	0.56
1:D:41:HIS:HE1	3:D:1001:HOH:O	1.82	0.56
1:B:74:HIS:N	1:B:74:HIS:HD2	2.03	0.56
1:A:93:SER:HA	1:A:96:ASN:HD21	1.70	0.56
1:C:157:THR:HG22	1:C:158:LYS:HG3	1.87	0.56
1:B:52:HIS:CA	1:B:74:HIS:N	2.62	0.56
1:C:139:LYS:CE	1:C:140:SER:O	2.54	0.56
1:B:179:ARG:HG3	1:B:179:ARG:HH11	1.70	0.55
1:B:138:ILE:C	1:B:139:LYS:HG2	2.32	0.55
1:C:139:LYS:HB3	1:C:140:SER:HB2	1.89	0.55
1:D:14:VAL:O	1:D:18:GLU:HG3	2.07	0.55
1:D:161:TYR:O	1:D:163:LEU:N	2.38	0.55
1:C:142:LYS:HB2	3:C:1004:HOH:O	2.06	0.54
1:B:41:HIS:HE1	1:B:80:GLU:OE1	1.91	0.54
1:A:107:PRO:HG2	1:A:117:PHE:CD2	2.43	0.54
1:C:19:LYS:O	1:C:23:GLU:HG2	2.07	0.54
1:D:152:GLY:O	1:D:172:LYS:HD2	2.08	0.54
1:D:179:ARG:HH11	1:D:179:ARG:HB3	1.73	0.54
1:A:124:ARG:HD3	1:A:191:PHE:CE2	2.43	0.54
1:C:107:PRO:HA	1:C:119:GLU:OE1	2.08	0.53
1:B:192:ARG:HH21	1:B:193:GLN:NE2	2.06	0.53
1:A:138:ILE:O	1:A:139:LYS:C	2.52	0.53
1:B:147:ILE:HD13	1:B:155:MET:O	2.09	0.53
1:D:79:ILE:HD13	1:D:107:PRO:HG2	1.91	0.53
1:D:-2:LEU:C	1:D:-2:LEU:HD23	2.34	0.53
1:D:108:ASP:O	1:D:109:LEU:HD23	2.09	0.53
1:D:140:SER:OG	1:D:142:LYS:HB2	2.08	0.53
1:A:88:TRP:CD2	1:A:106:LEU:HD21	2.44	0.53
1:C:43:GLU:HG3	1:C:47:MET:HE2	1.91	0.53
1:D:3:ASP:O	1:D:7:GLN:CD	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLU:O	1:C:22:LYS:HG3	2.09	0.52
1:A:31:GLU:HB3	1:A:34:LYS:CG	2.39	0.52
1:A:96:ASN:ND2	1:A:96:ASN:N	2.52	0.52
1:C:-2:LEU:HD12	1:C:-2:LEU:H1	1.75	0.52
1:D:98:THR:CG2	1:D:100:VAL:HG13	2.39	0.51
1:C:147:ILE:HD12	1:C:148:PHE:O	2.10	0.51
1:A:96:ASN:HD22	1:A:96:ASN:N	2.02	0.51
1:D:176:PHE:HE1	1:D:179:ARG:HH22	1.59	0.51
1:D:131:TYR:CE1	1:D:145:ILE:HB	2.45	0.51
1:D:4:PHE:CZ	1:D:182:MET:HG2	2.46	0.51
1:A:127:VAL:HG22	1:A:153:GLU:OE2	2.11	0.51
1:D:182:MET:HE2	1:D:188:TRP:CE3	2.42	0.51
1:B:43:GLU:HG3	1:B:47:MET:HE2	1.93	0.50
1:A:92:ASN:O	1:A:96:ASN:ND2	2.44	0.50
1:C:127:VAL:HG12	1:C:147:ILE:HD11	1.94	0.50
1:A:95:CYS:SG	1:A:102:LYS:HA	2.51	0.50
1:D:139:LYS:HB2	1:D:139:LYS:HZ2	1.76	0.50
1:D:192:ARG:CZ	1:D:192:ARG:HB3	2.41	0.50
1:D:188:TRP:NE1	1:D:192:ARG:NH1	2.60	0.50
1:D:75:ARG:NH2	1:D:113:LYS:HD3	2.27	0.49
1:A:138:ILE:HD11	1:A:145:ILE:HD11	1.93	0.49
1:B:92:ASN:HD21	1:B:102:LYS:CE	2.24	0.49
1:B:138:ILE:CG1	1:B:139:LYS:N	2.73	0.49
1:C:107:PRO:HG3	1:C:117:PHE:CD2	2.47	0.49
1:D:10:ASN:HD21	1:D:12:MET:HB2	1.78	0.49
1:D:182:MET:HE3	1:D:188:TRP:HA	1.94	0.49
1:B:184:SER:C	1:B:185:ARG:HD3	2.37	0.49
1:A:88:TRP:CE2	1:A:106:LEU:HD21	2.47	0.49
1:C:96:ASN:ND2	1:C:97:THR:HG23	2.27	0.49
1:A:21:MET:CE	1:A:34:LYS:HD3	2.41	0.49
1:A:2:GLU:OE1	1:A:29:LYS:HG2	2.13	0.49
1:D:139:LYS:NZ	1:D:139:LYS:CB	2.76	0.49
1:C:123:THR:HG22	1:C:147:ILE:CD1	2.41	0.48
1:D:141:GLU:CD	1:D:141:GLU:N	2.70	0.48
1:C:21:MET:HG2	1:C:38:ILE:CD1	2.44	0.48
1:C:193:GLN:HG2	3:C:1006:HOH:O	2.13	0.48
1:D:110:TYR:HA	1:D:117:PHE:HA	1.96	0.48
1:D:179:ARG:HG2	1:D:188:TRP:CE3	2.48	0.48
1:D:185:ARG:CD	1:D:187:LEU:HD22	2.44	0.48
1:D:137:LYS:C	1:D:139:LYS:H	2.20	0.48
1:C:174:ARG:O	1:C:178:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:HIS:CE1	1:D:160:ASP:HB3	2.49	0.47
1:B:78:ILE:HG12	1:B:109:LEU:CD2	2.43	0.47
1:D:179:ARG:HB3	1:D:179:ARG:NH1	2.30	0.47
1:B:41:HIS:CE1	1:B:80:GLU:OE1	2.67	0.47
1:D:147:ILE:HD13	1:D:155:MET:O	2.13	0.47
1:D:185:ARG:HD2	1:D:187:LEU:HD22	1.95	0.47
1:B:138:ILE:O	1:B:139:LYS:CG	2.62	0.47
1:D:124:ARG:O	1:D:192:ARG:HG3	2.14	0.47
1:A:117:PHE:HB2	1:A:143:THR:HG22	1.95	0.47
1:A:147:ILE:HD13	3:A:1031:HOH:O	2.14	0.47
1:B:86:MET:O	1:B:90:VAL:HG23	2.15	0.47
1:B:104:LYS:HD3	1:B:104:LYS:H	1.79	0.47
1:D:42:LEU:HD23	1:D:80:GLU:HG3	1.96	0.47
1:A:34:LYS:O	1:A:38:ILE:HG12	2.15	0.47
1:A:146:HIS:C	1:A:147:ILE:HD12	2.40	0.47
1:C:195:GLU:C	1:C:196:ARG:HG3	2.39	0.47
1:D:10:ASN:HD21	1:D:12:MET:HG3	1.79	0.47
1:D:34:LYS:O	1:D:38:ILE:HG13	2.15	0.47
1:A:147:ILE:HD12	1:A:147:ILE:N	2.30	0.47
1:A:93:SER:O	1:A:96:ASN:ND2	2.48	0.46
1:B:51:PHE:CE1	1:B:163:LEU:HD22	2.50	0.46
1:C:154:GLU:OE1	1:C:168:ARG:HD2	2.16	0.46
1:D:146:HIS:HE1	1:D:168:ARG:HD3	1.80	0.46
1:C:179:ARG:HG2	1:C:188:TRP:CE3	2.50	0.46
1:A:150:PHE:O	1:A:179:ARG:NH2	2.48	0.46
1:B:121:GLY:HA3	1:B:147:ILE:HG22	1.98	0.46
1:D:105:PHE:CD2	1:D:138:ILE:HG22	2.51	0.46
1:B:139:LYS:HB2	1:B:140:SER:H	1.19	0.46
1:D:92:ASN:HD21	1:D:102:LYS:HZ1	1.63	0.46
1:A:23:GLU:OE2	1:A:84:ARG:HD2	2.16	0.46
1:C:147:ILE:O	1:C:147:ILE:HG13	2.15	0.46
1:A:161:TYR:CD2	1:A:168:ARG:NH1	2.83	0.46
1:A:174:ARG:O	1:A:174:ARG:HD2	2.15	0.46
1:C:124:ARG:HD2	1:C:191:PHE:CZ	2.51	0.45
1:A:26:GLU:OE1	1:A:34:LYS:HE3	2.16	0.45
1:A:165:GLU:CD	1:A:168:ARG:HH21	2.24	0.45
1:D:174:ARG:NH1	1:D:178:ILE:HG22	2.31	0.45
1:B:185:ARG:HG3	1:B:185:ARG:NH1	2.31	0.45
1:B:77:GLU:HB3	1:B:110:TYR:HB3	1.97	0.45
1:C:123:THR:HG22	1:C:147:ILE:HD11	1.99	0.45
1:D:40:THR:CG2	1:D:122:VAL:HG11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:HG21	1:B:138:ILE:HD13	1.38	0.45
1:B:182:MET:SD	1:B:191:PHE:CD2	3.10	0.45
1:A:21:MET:HE3	1:A:34:LYS:HD3	1.98	0.45
1:A:75:ARG:HA	1:A:112:TYR:CE2	2.52	0.45
1:B:75:ARG:O	1:B:112:TYR:HD2	1.98	0.45
1:D:2:GLU:OE1	1:D:29:LYS:HD2	2.17	0.45
1:C:2:GLU:HG2	1:C:6:ARG:HE	1.82	0.45
1:C:94:ILE:O	1:C:95:CYS:C	2.59	0.45
1:B:176:PHE:HE1	1:B:180:GLN:OE1	2.00	0.45
1:C:116:ARG:HH22	1:C:162:THR:HG22	1.82	0.45
1:A:40:THR:O	1:A:44:VAL:HG23	2.17	0.44
1:C:138:ILE:HD12	1:C:140:SER:HB3	1.99	0.44
1:D:26:GLU:HG2	1:D:31:GLU:CD	2.42	0.44
1:D:137:LYS:C	1:D:139:LYS:N	2.75	0.44
1:B:96:ASN:HA	1:C:180:GLN:HE21	1.83	0.44
1:B:135:ALA:HA	1:B:145:ILE:HD11	1.99	0.44
1:C:1:MET:HE1	1:C:182:MET:HE2	1.99	0.44
1:A:101:GLU:OE2	1:A:142:LYS:HE3	2.18	0.44
1:B:176:PHE:CE1	1:B:180:GLN:OE1	2.71	0.44
1:B:1:MET:O	1:B:5:VAL:HG23	2.18	0.44
1:C:142:LYS:HD2	3:C:1004:HOH:O	2.16	0.44
1:D:79:ILE:CD1	1:D:107:PRO:HG2	2.47	0.44
1:D:151:THR:HB	1:D:153:GLU:OE1	2.17	0.44
1:D:126:GLU:OE2	1:D:128:HIS:HB3	2.18	0.44
1:D:157:THR:HG22	1:D:158:LYS:HG2	2.00	0.44
1:B:105:PHE:CD2	1:B:106:LEU:N	2.85	0.44
1:B:131:TYR:CE1	1:B:145:ILE:HB	2.52	0.44
1:B:179:ARG:NH1	1:B:188:TRP:CZ2	2.85	0.44
1:D:19:LYS:O	1:D:23:GLU:HB2	2.18	0.44
1:D:177:THR:C	1:D:179:ARG:N	2.76	0.44
1:A:31:GLU:HB3	1:A:34:LYS:HD2	1.99	0.43
1:A:10:ASN:ND2	1:A:12:MET:CB	2.81	0.43
1:A:93:SER:CA	1:A:96:ASN:HD21	2.30	0.43
1:D:10:ASN:ND2	1:D:12:MET:HB2	2.32	0.43
1:A:47:MET:HE1	1:A:174:ARG:HB3	2.00	0.43
1:D:135:ALA:HB2	1:D:145:ILE:HD12	1.99	0.43
1:A:10:ASN:HB3	1:A:13:ILE:HG12	2.01	0.43
1:A:107:PRO:HG2	1:A:117:PHE:CG	2.53	0.43
1:C:-2:LEU:N	1:C:-2:LEU:CD1	2.82	0.43
1:D:10:ASN:HD21	1:D:12:MET:CB	2.31	0.43
1:C:139:LYS:CD	1:C:140:SER:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:PHE:O	1:D:194:SER:OG	2.34	0.43
1:B:140:SER:C	1:B:142:LYS:H	2.26	0.43
1:C:176:PHE:CD1	1:C:179:ARG:NH2	2.87	0.43
1:D:185:ARG:HG3	1:D:187:LEU:HD22	2.00	0.43
1:C:127:VAL:HG23	1:C:128:HIS:N	2.34	0.42
1:D:17:ALA:O	1:D:21:MET:HG3	2.19	0.42
1:D:134:LYS:O	1:D:138:ILE:HD13	2.19	0.42
1:C:122:VAL:HA	1:C:148:PHE:O	2.19	0.42
1:D:183:ALA:C	1:D:185:ARG:H	2.26	0.42
1:C:94:ILE:HD13	1:C:110:TYR:CG	2.54	0.42
1:D:125:ARG:HB2	1:D:126:GLU:H	1.56	0.42
1:A:161:TYR:CG	1:A:168:ARG:NH1	2.87	0.42
1:B:10:ASN:ND2	1:B:12:MET:HB3	2.34	0.42
1:C:30:ILE:HD13	1:C:30:ILE:H	1.84	0.42
1:C:21:MET:HE1	1:C:31:GLU:HB2	2.02	0.42
1:D:134:LYS:HB3	1:D:145:ILE:HD13	2.01	0.42
1:A:1:MET:HB2	1:C:165:GLU:HG3	2.02	0.42
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.85	0.42
1:D:158:LYS:HE2	1:D:158:LYS:CA	2.47	0.42
1:A:166:GLU:O	1:A:170:ARG:HD3	2.20	0.42
1:B:10:ASN:HD22	1:B:12:MET:HB3	1.84	0.42
1:D:26:GLU:HG2	1:D:31:GLU:OE2	2.20	0.42
1:B:181:GLU:O	1:B:185:ARG:HG2	2.19	0.42
1:B:179:ARG:HG3	1:B:179:ARG:NH1	2.34	0.42
1:A:128:HIS:CD2	1:A:155:MET:HE1	2.54	0.41
1:A:1:MET:CE	1:A:182:MET:HE2	2.47	0.41
1:C:161:TYR:O	1:C:163:LEU:N	2.53	0.41
1:B:138:ILE:HG13	1:B:140:SER:HB2	2.03	0.41
1:B:147:ILE:HD13	1:B:147:ILE:N	2.30	0.41
1:D:102:LYS:HE3	1:D:102:LYS:HB2	1.82	0.41
1:B:176:PHE:O	1:B:180:GLN:HG2	2.20	0.41
1:C:87:ALA:O	1:C:90:VAL:HG23	2.20	0.41
1:D:177:THR:C	1:D:179:ARG:H	2.28	0.41
1:A:158:LYS:O	1:A:159:ALA:HB3	2.20	0.41
1:B:10:ASN:ND2	1:B:12:MET:H	2.19	0.41
1:C:42:LEU:O	1:C:46:PHE:HD2	2.03	0.41
1:C:116:ARG:HH12	1:C:162:THR:CG2	2.34	0.41
1:A:83:ASP:CG	1:B:85:THR:HB	2.46	0.41
1:B:94:ILE:HA	1:B:97:THR:CG2	2.50	0.41
1:D:174:ARG:CZ	1:D:178:ILE:HG22	2.51	0.41
1:A:185:ARG:O	1:A:187:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:C	1:B:169:ALA:N	2.76	0.40
1:D:-2:LEU:HD23	1:D:-1:GLY:O	2.21	0.40
1:A:10:ASN:ND2	1:A:12:MET:HB3	2.36	0.40
1:C:193:GLN:NE2	3:C:1005:HOH:O	2.54	0.40
1:B:10:ASN:HB3	1:B:13:ILE:HD12	2.04	0.40
1:B:96:ASN:O	1:C:179:ARG:NH1	2.54	0.40
1:D:49:SER:OG	1:D:78:ILE:HD11	2.21	0.40
1:D:181:GLU:HA	1:D:181:GLU:OE1	2.20	0.40
1:A:2:GLU:HB2	1:A:32:THR:HG21	2.02	0.40
1:A:17:ALA:O	1:A:21:MET:HG3	2.21	0.40
1:D:131:TYR:HB2	1:D:147:ILE:HD12	2.03	0.40
1:A:2:GLU:CD	1:A:29:LYS:HG2	2.47	0.40
1:D:-2:LEU:C	1:D:-2:LEU:CD2	2.95	0.40
1:D:40:THR:HG22	1:D:122:VAL:HG11	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	171/259 (66%)	159 (93%)	11 (6%)	1 (1%)	21	23
1	B	171/259 (66%)	159 (93%)	8 (5%)	4 (2%)	5	3
1	C	172/259 (66%)	155 (90%)	13 (8%)	4 (2%)	5	3
1	D	171/259 (66%)	154 (90%)	13 (8%)	4 (2%)	5	3
All	All	685/1036 (66%)	627 (92%)	45 (7%)	13 (2%)	6	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	THR

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Mol	Chain	Res	Type
1	B	139	LYS
1	B	140	SER
1	C	139	LYS
1	C	162	THR
1	B	75	ARG
1	D	115	ASN
1	A	162	THR
1	B	137	LYS
1	C	98	THR
1	C	140	SER
1	D	184	SER
1	D	138	ILE

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	157/231 (68%)	144 (92%)	13 (8%)	10	11
1	B	159/231 (69%)	143 (90%)	16 (10%)	7	7
1	C	158/231 (68%)	143 (90%)	15 (10%)	8	8
1	D	157/231 (68%)	142 (90%)	15 (10%)	8	8
All	All	631/924 (68%)	572 (91%)	59 (9%)	8	9

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	34	LYS
1	A	93	SER
1	A	96	ASN
1	A	101	GLU
1	A	104	LYS
1	A	112	TYR
1	A	141	GLU
1	A	142	LYS

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Mol	Chain	Res	Type
1	A	173	THR
1	A	180	GLN
1	A	187	LEU
1	A	189	ASP
1	B	7	GLN
1	B	15	GLU
1	B	74	HIS
1	B	101	GLU
1	B	104	LYS
1	B	113	LYS
1	B	126	GLU
1	B	137	LYS
1	B	141	GLU
1	B	143	THR
1	B	147	ILE
1	B	162	THR
1	B	172	LYS
1	B	173	THR
1	B	185	ARG
1	B	187	LEU
1	C	-2	LEU
1	C	7	GLN
1	C	12	MET
1	C	24	TYR
1	C	30	ILE
1	C	43	GLU
1	C	90	VAL
1	C	100	VAL
1	C	104	LYS
1	C	140	SER
1	C	141	GLU
1	C	142	LYS
1	C	147	ILE
1	C	170	ARG
1	C	187	LEU
1	D	7	GLN
1	D	26	GLU
1	D	43	GLU
1	D	84	ARG
1	D	104	LYS
1	D	119	GLU
1	D	137	LYS

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Mol	Chain	Res	Type
1	D	138	ILE
1	D	139	LYS
1	D	147	ILE
1	D	151	THR
1	D	162	THR
1	D	179	ARG
1	D	181	GLU
1	D	187	LEU

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	10	ASN
1	A	92	ASN
1	A	96	ASN
1	A	136	ASN
1	A	193	GLN
1	B	7	GLN
1	B	10	ASN
1	B	33	ASN
1	B	52	HIS
1	B	74	HIS
1	B	92	ASN
1	B	193	GLN
1	C	7	GLN
1	C	92	ASN
1	C	96	ASN
1	C	128	HIS
1	D	10	ASN
1	D	92	ASN
1	D	96	ASN
1	D	128	HIS
1	D	136	ASN
1	D	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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	175/259 (67%)	-0.29	1 (0%) 85 83	25, 45, 62, 69	0
1	B	175/259 (67%)	-0.17	0 100 100	28, 47, 66, 81	0
1	C	176/259 (67%)	-0.13	1 (0%) 85 83	31, 52, 68, 83	0
1	D	175/259 (67%)	-0.02	0 100 100	33, 52, 75, 94	0
All	All	701/1036 (67%)	-0.15	2 (0%) 90 88	25, 48, 69, 94	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	TYR	2.4
1	C	105	PHE	2.1

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	MG	D	999	1/1	0.71	0.20	67,67,67,67	0
2	MG	A	999	1/1	0.93	0.10	45,45,45,45	0
2	MG	C	999	1/1	0.94	0.10	46,46,46,46	0
2	MG	B	999	1/1	0.95	0.10	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.