



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:54 AM UTC

PDB ID : 8G6D / pdb_00008g6d
Title : HSV-1 Nuclear Egress Complex (SUP; UL31-R229L)
Authors : Draganova, E.B.; Gonzalez Del-Pino, G.L.; Heldwein, E.E.
Deposited on : 2023-02-15
Resolution : 3.92 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

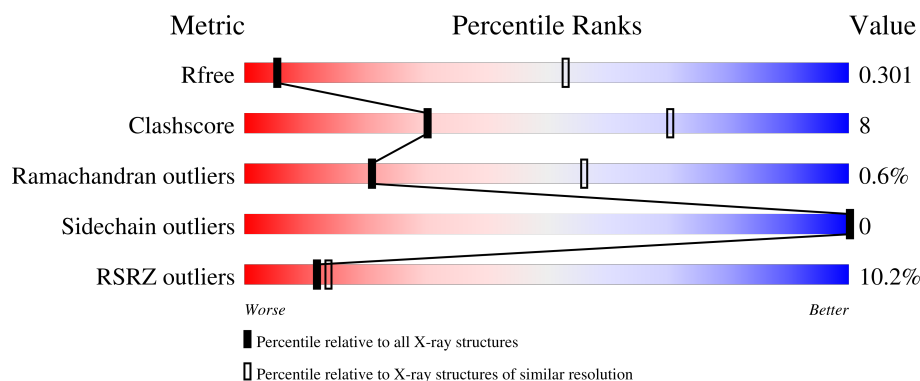
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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	183	10% 75% 15% 10%
1	C	183	10% 69% 21% 10%
1	E	183	9% 72% 19% 10%
1	G	183	10% 68% 21% 11%
1	I	183	12% 66% 23% 11%

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Mol	Chain	Length	Quality of chain
1	K	183	7% 73% 16% 10%
2	B	260	9% 78% 18%
2	D	260	12% 78% 19%
2	F	260	8% 77% 20%
2	H	260	8% 78% 18%
2	J	260	10% 75% 20%
2	L	260	10% 78% 18% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19341 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 Virion egress protein UL34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1277	806	231	231	9			
1	C	165	Total	C	N	O	S	0	0	0
			1277	806	231	231	9			
1	E	165	Total	C	N	O	S	0	0	0
			1277	806	231	231	9			
1	G	163	Total	C	N	O	S	0	0	0
			1259	796	226	228	9			
1	I	163	Total	C	N	O	S	0	0	0
			1259	796	226	228	9			
1	K	164	Total	C	N	O	S	0	0	0
			1266	800	227	230	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P10218
A	4	PRO	-	expression tag	UNP P10218
A	5	LEU	-	expression tag	UNP P10218
A	6	GLY	-	expression tag	UNP P10218
A	7	SER	-	expression tag	UNP P10218
A	8	PRO	-	expression tag	UNP P10218
A	9	GLU	-	expression tag	UNP P10218
A	10	PHE	-	expression tag	UNP P10218
A	11	PRO	-	expression tag	UNP P10218
A	12	GLY	-	expression tag	UNP P10218
A	13	ARG	-	expression tag	UNP P10218
A	14	PRO	-	expression tag	UNP P10218
C	3	GLY	-	expression tag	UNP P10218
C	4	PRO	-	expression tag	UNP P10218
C	5	LEU	-	expression tag	UNP P10218
C	6	GLY	-	expression tag	UNP P10218
C	7	SER	-	expression tag	UNP P10218

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	PRO	-	expression tag	UNP P10218
C	9	GLU	-	expression tag	UNP P10218
C	10	PHE	-	expression tag	UNP P10218
C	11	PRO	-	expression tag	UNP P10218
C	12	GLY	-	expression tag	UNP P10218
C	13	ARG	-	expression tag	UNP P10218
C	14	PRO	-	expression tag	UNP P10218
E	3	GLY	-	expression tag	UNP P10218
E	4	PRO	-	expression tag	UNP P10218
E	5	LEU	-	expression tag	UNP P10218
E	6	GLY	-	expression tag	UNP P10218
E	7	SER	-	expression tag	UNP P10218
E	8	PRO	-	expression tag	UNP P10218
E	9	GLU	-	expression tag	UNP P10218
E	10	PHE	-	expression tag	UNP P10218
E	11	PRO	-	expression tag	UNP P10218
E	12	GLY	-	expression tag	UNP P10218
E	13	ARG	-	expression tag	UNP P10218
E	14	PRO	-	expression tag	UNP P10218
G	3	GLY	-	expression tag	UNP P10218
G	4	PRO	-	expression tag	UNP P10218
G	5	LEU	-	expression tag	UNP P10218
G	6	GLY	-	expression tag	UNP P10218
G	7	SER	-	expression tag	UNP P10218
G	8	PRO	-	expression tag	UNP P10218
G	9	GLU	-	expression tag	UNP P10218
G	10	PHE	-	expression tag	UNP P10218
G	11	PRO	-	expression tag	UNP P10218
G	12	GLY	-	expression tag	UNP P10218
G	13	ARG	-	expression tag	UNP P10218
G	14	PRO	-	expression tag	UNP P10218
I	3	GLY	-	expression tag	UNP P10218
I	4	PRO	-	expression tag	UNP P10218
I	5	LEU	-	expression tag	UNP P10218
I	6	GLY	-	expression tag	UNP P10218
I	7	SER	-	expression tag	UNP P10218
I	8	PRO	-	expression tag	UNP P10218
I	9	GLU	-	expression tag	UNP P10218
I	10	PHE	-	expression tag	UNP P10218
I	11	PRO	-	expression tag	UNP P10218
I	12	GLY	-	expression tag	UNP P10218
I	13	ARG	-	expression tag	UNP P10218

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Chain	Residue	Modelled	Actual	Comment	Reference
I	14	PRO	-	expression tag	UNP P10218
K	3	GLY	-	expression tag	UNP P10218
K	4	PRO	-	expression tag	UNP P10218
K	5	LEU	-	expression tag	UNP P10218
K	6	GLY	-	expression tag	UNP P10218
K	7	SER	-	expression tag	UNP P10218
K	8	PRO	-	expression tag	UNP P10218
K	9	GLU	-	expression tag	UNP P10218
K	10	PHE	-	expression tag	UNP P10218
K	11	PRO	-	expression tag	UNP P10218
K	12	GLY	-	expression tag	UNP P10218
K	13	ARG	-	expression tag	UNP P10218
K	14	PRO	-	expression tag	UNP P10218

- Molecule 2 is a protein called Nuclear egress protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	253	Total	C	N	O	S	0	0	0
			1967	1267	335	351	14			
2	D	253	Total	C	N	O	S	0	0	0
			1967	1267	335	351	14			
2	F	253	Total	C	N	O	S	0	0	0
			1967	1267	335	351	14			
2	H	250	Total	C	N	O	S	0	0	0
			1946	1252	332	348	14			
2	J	250	Total	C	N	O	S	0	0	0
			1943	1252	330	348	13			
2	L	248	Total	C	N	O	S	0	0	0
			1928	1243	327	344	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	GLY	-	expression tag	UNP P10215
B	48	PRO	-	expression tag	UNP P10215
B	49	GLY	-	expression tag	UNP P10215
B	50	SER	-	expression tag	UNP P10215
B	229	LEU	ARG	conflict	UNP P10215
D	47	GLY	-	expression tag	UNP P10215
D	48	PRO	-	expression tag	UNP P10215
D	49	GLY	-	expression tag	UNP P10215
D	50	SER	-	expression tag	UNP P10215

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Chain	Residue	Modelled	Actual	Comment	Reference
D	229	LEU	ARG	conflict	UNP P10215
F	47	GLY	-	expression tag	UNP P10215
F	48	PRO	-	expression tag	UNP P10215
F	49	GLY	-	expression tag	UNP P10215
F	50	SER	-	expression tag	UNP P10215
F	229	LEU	ARG	conflict	UNP P10215
H	47	GLY	-	expression tag	UNP P10215
H	48	PRO	-	expression tag	UNP P10215
H	49	GLY	-	expression tag	UNP P10215
H	50	SER	-	expression tag	UNP P10215
H	229	LEU	ARG	conflict	UNP P10215
J	47	GLY	-	expression tag	UNP P10215
J	48	PRO	-	expression tag	UNP P10215
J	49	GLY	-	expression tag	UNP P10215
J	50	SER	-	expression tag	UNP P10215
J	229	LEU	ARG	conflict	UNP P10215
L	47	GLY	-	expression tag	UNP P10215
L	48	PRO	-	expression tag	UNP P10215
L	49	GLY	-	expression tag	UNP P10215
L	50	SER	-	expression tag	UNP P10215
L	229	LEU	ARG	conflict	UNP P10215

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0

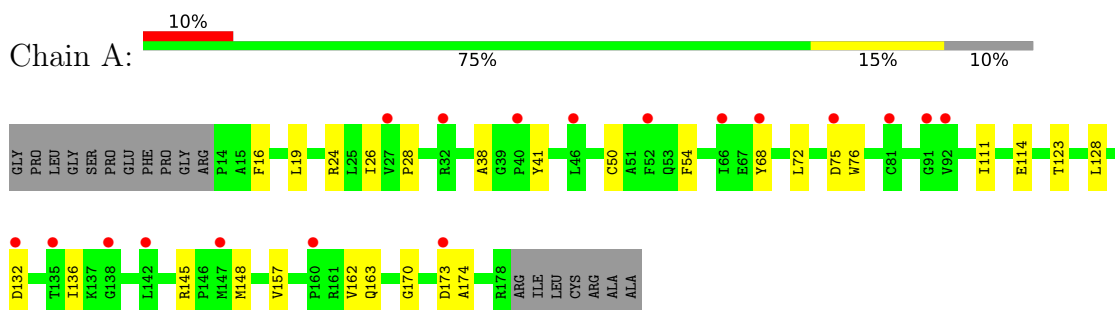
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	O 1	0	0
4	J	1	Total 1	O 1	0	0

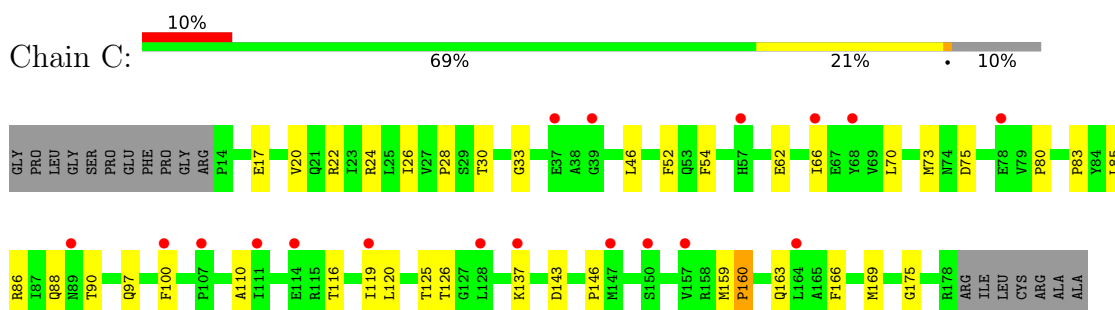
3 Residue-property plots [i](#)

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.

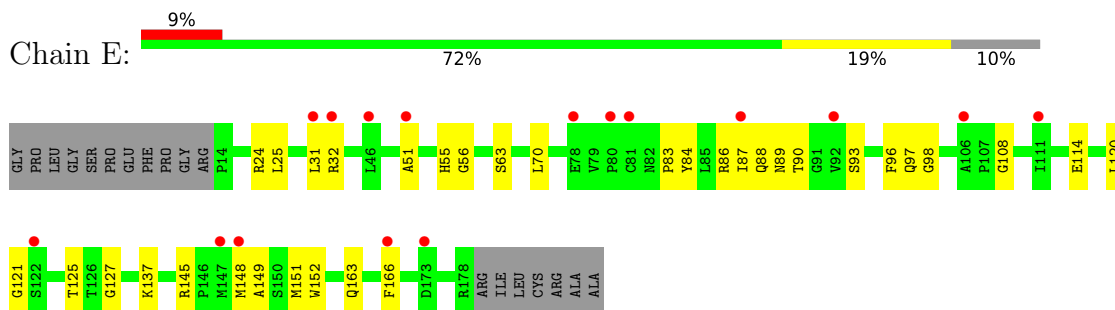
- Molecule 1: Virion egress protein UL34



- Molecule 1: Virion egress protein UL34

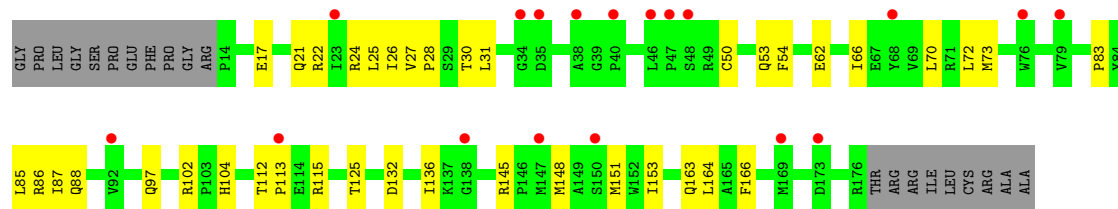


- Molecule 1: Virion egress protein UL34

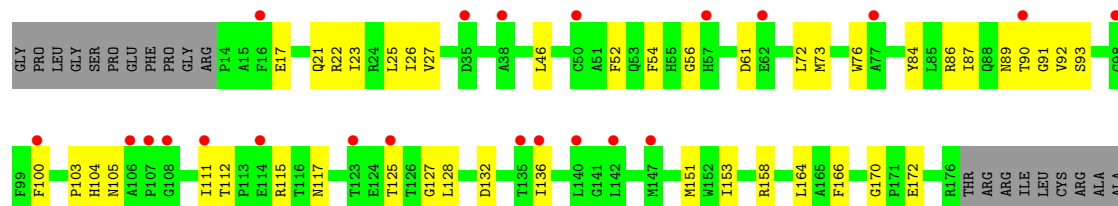


- Molecule 1: Virion egress protein UL34

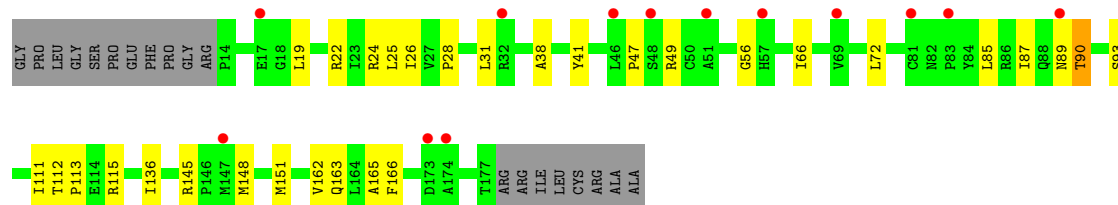
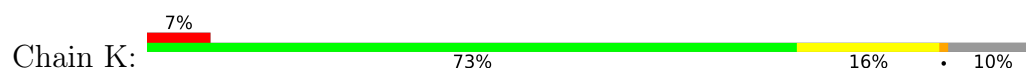




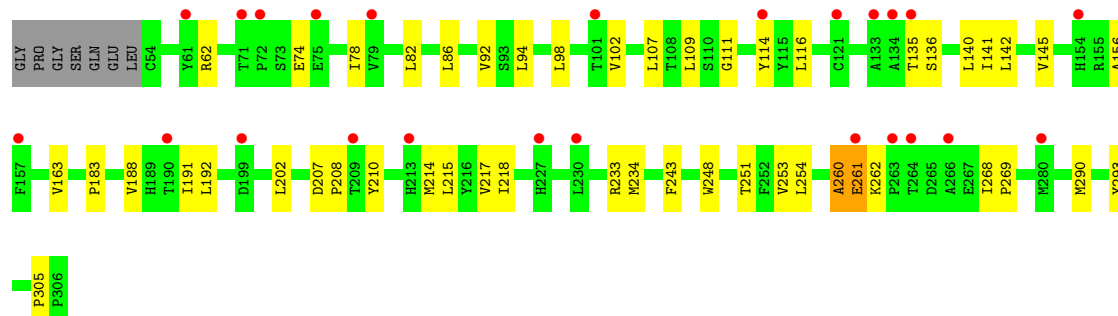
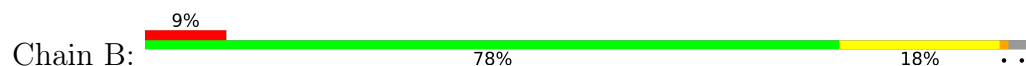
• Molecule 1: Virion egress protein UL34



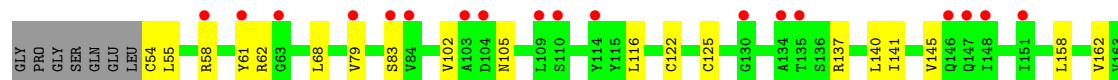
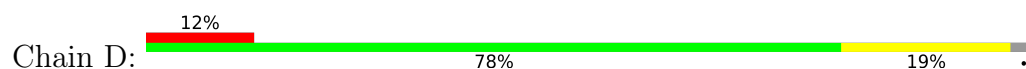
• Molecule 1: Virion egress protein UL34

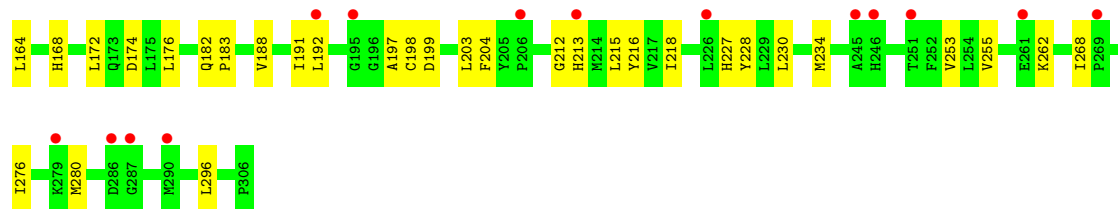


• Molecule 2: Nuclear egress protein 1

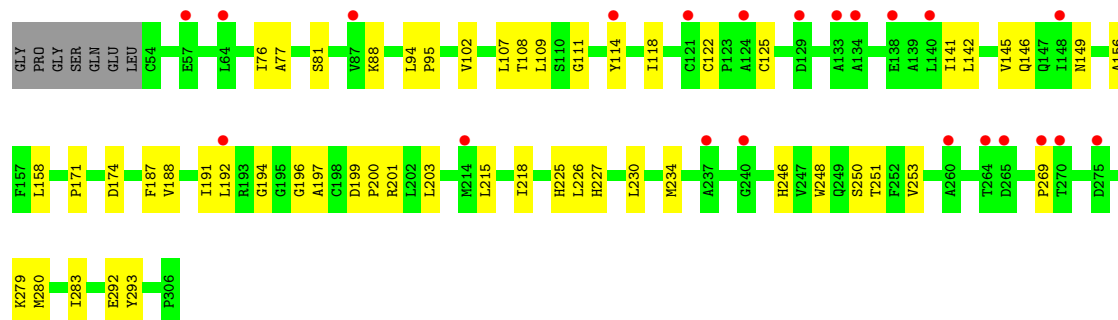
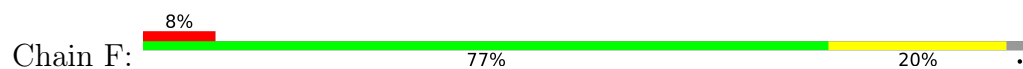


• Molecule 2: Nuclear egress protein 1

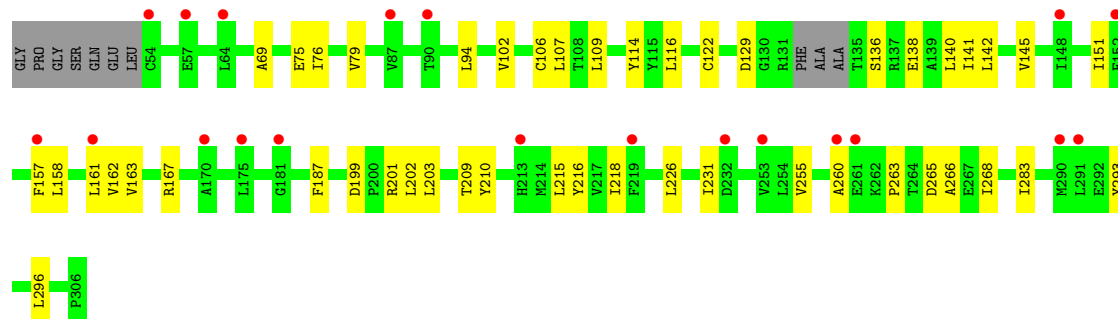
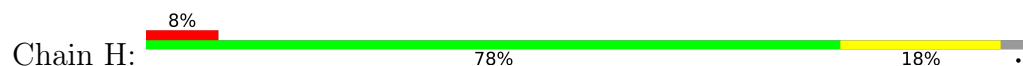




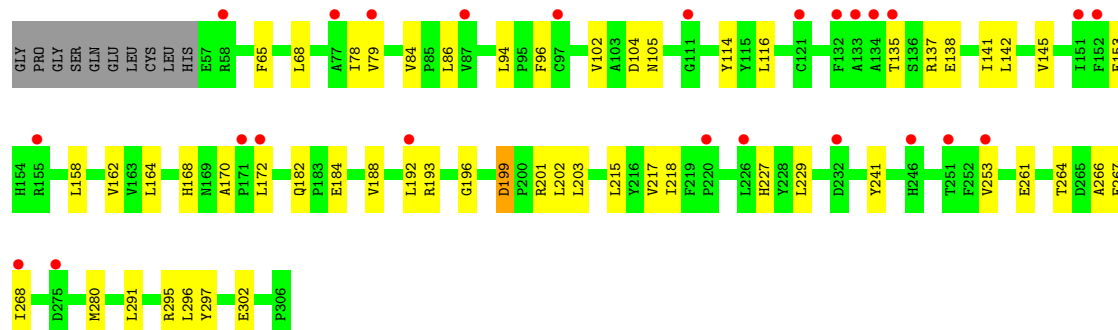
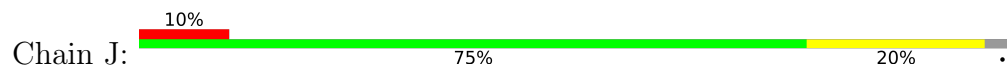
• Molecule 2: Nuclear egress protein 1



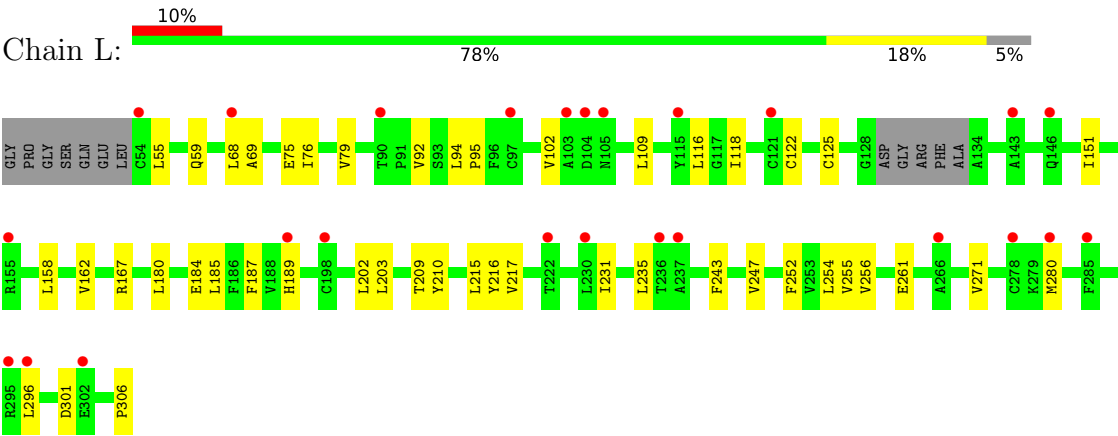
• Molecule 2: Nuclear egress protein 1



• Molecule 2: Nuclear egress protein 1



• Molecule 2: Nuclear egress protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.56Å 189.10Å 157.10Å 90.00° 100.52° 90.00°	Depositor
Resolution (Å)	94.55 – 3.92 94.55 – 3.92	Depositor EDS
% Data completeness (in resolution range)	97.9 (94.55-3.92) 84.9 (94.55-3.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.255 , 0.301 0.255 , 0.301	Depositor DCC
R_{free} test set	1990 reflections (7.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	19341	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.17	0/1311	0.48	0/1777
1	C	0.15	0/1311	0.41	0/1777
1	E	0.14	0/1311	0.35	0/1777
1	G	0.15	0/1293	0.40	0/1753
1	I	0.17	0/1293	0.41	0/1753
1	K	0.14	0/1300	0.36	0/1763
2	B	0.16	0/2019	0.40	0/2750
2	D	0.15	0/2019	0.40	0/2750
2	F	0.15	0/2019	0.44	2/2750 (0.1%)
2	H	0.17	0/1996	0.44	0/2717
2	J	0.16	0/1994	0.44	0/2716
2	L	0.15	0/1978	0.38	0/2694
All	All	0.16	0/19844	0.41	2/26977 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	194	GLY	CA-C-N	5.35	131.16	120.77
2	F	194	GLY	C-N-CA	5.35	131.16	120.77

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1277	0	1251	21	0
1	C	1277	0	1251	28	0
1	E	1277	0	1251	21	0
1	G	1259	0	1231	26	0
1	I	1259	0	1231	35	0
1	K	1266	0	1238	27	0
2	B	1967	0	1947	35	0
2	D	1967	0	1947	36	0
2	F	1967	0	1947	34	0
2	H	1946	0	1927	30	0
2	J	1943	0	1924	38	0
2	L	1928	0	1912	34	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	D	1	0	0	0	0
4	J	1	0	0	0	0
All	All	19341	0	19057	323	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 8.

All (323) 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)
2:B:145:VAL:HG12	2:B:269:PRO:HG3	1.55	0.87
2:D:183:PRO:HG3	2:D:268:ILE:HG21	1.59	0.83
2:J:158:LEU:HB3	2:J:280:MET:HE3	1.66	0.78
1:A:163:GLN:HB3	2:B:102:VAL:HG12	1.65	0.76
1:K:26:ILE:HD12	2:L:79:VAL:HG21	1.70	0.72
1:C:163:GLN:HB3	2:D:102:VAL:HG12	1.72	0.71
1:K:24:ARG:NH2	1:K:28:PRO:O	2.25	0.69
2:D:158:LEU:HB3	2:D:280:MET:HE3	1.72	0.69
1:G:26:ILE:HG23	2:H:79:VAL:HG11	1.75	0.69
1:C:46:LEU:HD13	1:C:100:PHE:HD2	1.57	0.69
1:G:24:ARG:NH1	1:G:31:LEU:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:CYS:SG	2:F:125:CYS:HB2	2.32	0.68
1:G:66:ILE:HG13	1:G:85:LEU:HD12	1.76	0.68
2:B:183:PRO:HG3	2:B:268:ILE:HG21	1.76	0.67
1:E:151:MET:HE2	1:E:166:PHE:HB3	1.75	0.67
2:B:202:LEU:HD22	2:B:215:LEU:HD21	1.77	0.67
1:C:137:LYS:NZ	1:C:143:ASP:O	2.28	0.66
1:G:70:LEU:HD21	1:G:85:LEU:HG	1.78	0.65
2:J:168:HIS:ND1	2:J:170:ALA:HB2	2.13	0.64
2:B:92:VAL:HG21	2:B:116:LEU:HG	1.79	0.64
1:K:163:GLN:HB3	2:L:102:VAL:HG12	1.79	0.64
1:C:88:GLN:HB2	1:C:125:THR:HG22	1.80	0.63
2:F:158:LEU:HB3	2:F:280:MET:HE3	1.80	0.63
1:I:151:MET:HE3	1:I:166:PHE:HB3	1.80	0.63
2:L:167:ARG:NH2	2:L:301:ASP:OD2	2.32	0.63
2:B:261:GLU:O	2:J:302:GLU:HG3	1.98	0.63
2:J:261:GLU:O	2:J:261:GLU:HG3	1.99	0.63
1:C:24:ARG:NH2	1:C:28:PRO:O	2.31	0.62
2:B:145:VAL:CG1	2:B:269:PRO:HG3	2.28	0.62
2:B:214:MET:HE1	2:B:305:PRO:HB3	1.81	0.62
1:G:73:MET:HE3	1:G:83:PRO:HB3	1.82	0.62
2:B:141:ILE:O	2:B:145:VAL:HG13	2.00	0.62
1:G:88:GLN:HB2	1:G:125:THR:HG22	1.82	0.61
1:G:86:ARG:NH2	1:G:97:GLN:OE1	2.33	0.61
2:J:203:LEU:HD11	2:J:296:LEU:HB3	1.82	0.60
2:F:279:LYS:O	2:F:283:ILE:HG12	2.02	0.60
2:B:260:ALA:O	2:B:262:LYS:N	2.35	0.59
2:J:104:ASP:O	2:J:105:ASN:ND2	2.35	0.59
2:H:209:THR:OG1	2:H:210:TYR:N	2.32	0.59
2:F:125:CYS:SG	2:F:225:HIS:CE1	2.96	0.58
1:C:169:MET:HE3	2:D:83:SER:HA	1.84	0.58
1:I:103:PRO:O	1:I:105:ASN:N	2.36	0.58
1:G:112:THR:HG22	1:G:115:ARG:HB3	1.85	0.58
1:G:17:GLU:O	1:G:21:GLN:HG3	2.03	0.58
2:J:138:GLU:O	2:J:142:LEU:HG	2.04	0.57
1:E:163:GLN:HB3	2:F:102:VAL:HG22	1.87	0.57
1:A:24:ARG:NH2	1:A:28:PRO:O	2.38	0.57
1:I:103:PRO:C	1:I:105:ASN:H	2.13	0.57
1:G:87:ILE:HG21	1:G:164:LEU:HD11	1.87	0.57
2:H:158:LEU:O	2:H:162:VAL:HG23	2.05	0.56
2:F:94:LEU:HD22	2:F:114:TYR:CE2	2.40	0.56
2:L:189:HIS:HD2	2:L:202:LEU:HD12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:87:ILE:HG21	1:I:164:LEU:HD11	1.87	0.56
2:D:212:GLY:O	2:D:213:HIS:ND1	2.38	0.56
2:B:142:LEU:O	2:B:145:VAL:HG22	2.06	0.55
2:F:114:TYR:OH	1:I:90:THR:O	2.18	0.55
2:D:203:LEU:HD11	2:D:296:LEU:HB3	1.87	0.55
1:A:38:ALA:HB2	1:A:50:CYS:O	2.07	0.55
2:B:243:PHE:HD2	2:B:254:LEU:HD21	1.72	0.55
2:J:268:ILE:O	2:J:268:ILE:HG13	2.06	0.55
2:H:203:LEU:HD11	2:H:296:LEU:HB3	1.89	0.55
1:G:66:ILE:HD12	1:G:153:ILE:HD11	1.88	0.54
1:K:66:ILE:HD13	1:K:85:LEU:HD22	1.88	0.54
2:J:201:ARG:HB2	2:J:218:ILE:HB	1.90	0.54
2:J:264:THR:HG23	2:J:266:ALA:H	1.71	0.54
2:J:184:GLU:O	2:J:188:VAL:HG23	2.07	0.54
1:I:170:GLY:N	2:J:84:VAL:O	2.38	0.54
2:J:68:LEU:HD21	2:J:78:ILE:HD12	1.89	0.54
1:G:151:MET:HE3	1:G:166:PHE:HD2	1.71	0.53
1:G:113:PRO:HD3	1:G:136:ILE:HD12	1.90	0.53
2:D:188:VAL:HG13	2:D:234:MET:HE3	1.89	0.53
2:J:201:ARG:HD2	2:J:296:LEU:HD11	1.89	0.53
1:K:26:ILE:HG23	2:L:79:VAL:HG11	1.90	0.53
1:I:46:LEU:HD11	1:I:76:TRP:HZ3	1.74	0.53
2:B:114:TYR:OH	1:K:90:THR:O	2.25	0.53
1:I:117:ASN:ND2	2:J:105:ASN:OD1	2.42	0.53
2:L:243:PHE:HB3	2:L:254:LEU:HD11	1.89	0.52
2:F:187:PHE:O	2:F:191:ILE:HG13	2.09	0.52
1:G:87:ILE:HD11	1:G:153:ILE:HD13	1.92	0.52
1:I:52:PHE:HE2	1:I:73:MET:HE2	1.74	0.52
1:E:88:GLN:HG3	1:E:125:THR:HG22	1.92	0.52
1:G:25:LEU:HD21	2:H:76:ILE:HD11	1.92	0.52
1:I:172:GLU:HG2	2:J:84:VAL:CG2	2.40	0.52
1:E:89:ASN:ND2	1:E:121:GLY:O	2.43	0.52
1:K:56:GLY:O	1:K:93:SER:OG	2.16	0.52
2:F:188:VAL:HG13	2:F:234:MET:HE3	1.92	0.52
1:A:114:GLU:HG3	1:K:49:ARG:HH12	1.75	0.51
2:B:188:VAL:HG13	2:B:234:MET:HE3	1.91	0.51
2:L:203:LEU:HD11	2:L:296:LEU:HB3	1.92	0.51
1:A:26:ILE:HD13	1:A:68:TYR:CE1	2.45	0.51
2:F:109:LEU:HD22	2:F:114:TYR:HD2	1.76	0.51
1:K:111:ILE:HG21	1:K:166:PHE:CG	2.45	0.51
1:E:145:ARG:HB2	1:E:148:MET:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HD11	1:A:72:LEU:HG	1.92	0.51
2:B:156:ALA:HB1	2:B:293:TYR:OH	2.11	0.51
1:C:119:ILE:HD12	1:C:163:GLN:HG2	1.92	0.51
2:D:158:LEU:O	2:D:162:VAL:HG23	2.11	0.51
1:C:90:THR:O	2:H:114:TYR:OH	2.26	0.51
1:I:56:GLY:O	1:I:93:SER:HB2	2.10	0.51
2:D:203:LEU:HD12	2:D:218:ILE:HD11	1.93	0.51
2:H:136:SER:O	2:H:140:LEU:HG	2.10	0.51
1:I:61:ASP:OD2	1:I:158:ARG:NH2	2.43	0.51
2:H:202:LEU:HG	2:H:215:LEU:HD11	1.92	0.50
2:L:185:LEU:HD22	2:L:215:LEU:HD23	1.93	0.50
2:H:265:ASP:OD1	2:H:266:ALA:N	2.45	0.50
2:L:122:CYS:HB3	2:L:125:CYS:HB2	1.93	0.50
2:D:192:LEU:HD23	2:D:230:LEU:HD23	1.92	0.50
1:G:22:ARG:NH1	2:H:69:ALA:HB2	2.26	0.50
1:C:116:THR:OG1	1:C:166:PHE:O	2.29	0.50
1:C:86:ARG:NH2	1:C:88:GLN:OE1	2.40	0.50
2:F:196:GLY:N	2:F:199:ASP:HB2	2.27	0.50
1:I:26:ILE:HG23	2:J:79:VAL:HG21	1.94	0.50
2:D:203:LEU:O	2:D:215:LEU:HD12	2.12	0.50
1:I:153:ILE:HG12	1:I:166:PHE:HD1	1.77	0.50
2:F:250:SER:HB3	1:I:92:VAL:HG23	1.92	0.50
2:J:94:LEU:HD12	2:J:114:TYR:CZ	2.47	0.50
2:H:138:GLU:O	2:H:142:LEU:HG	2.11	0.49
2:J:182:GLN:OE1	2:J:241:TYR:OH	2.29	0.49
2:L:109:LEU:HB3	2:L:252:PHE:CE1	2.47	0.49
2:D:227:HIS:HD1	2:D:228:TYR:N	2.11	0.49
2:F:171:PRO:HG2	2:F:174:ASP:HB3	1.95	0.49
1:E:24:ARG:NH1	1:E:31:LEU:O	2.46	0.48
1:A:145:ARG:HB2	1:A:148:MET:HG3	1.95	0.48
2:B:135:THR:HG21	2:B:191:ILE:HG12	1.95	0.48
2:F:141:ILE:HG23	2:F:269:PRO:HG3	1.95	0.48
1:I:89:ASN:C	1:I:91:GLY:H	2.20	0.48
2:J:202:LEU:HB3	2:J:215:LEU:HD11	1.95	0.48
2:D:197:ALA:O	2:D:199:ASP:N	2.46	0.48
1:A:132:ASP:O	1:A:136:ILE:HG12	2.14	0.48
1:K:151:MET:HE3	1:K:166:PHE:HD2	1.77	0.48
1:K:115:ARG:O	1:K:115:ARG:HG3	2.13	0.48
1:C:46:LEU:HD13	1:C:100:PHE:CD2	2.44	0.48
2:B:191:ILE:HG21	2:B:234:MET:HG3	1.95	0.48
2:D:105:ASN:HD21	2:D:116:LEU:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:PRO:HA	2:D:55:LEU:HD11	1.95	0.48
1:G:30:THR:HB	1:G:62:GLU:HG3	1.96	0.48
2:L:243:PHE:CD2	2:L:256:VAL:HG22	2.49	0.47
2:B:248:TRP:O	2:B:251:THR:OG1	2.25	0.47
2:J:158:LEU:O	2:J:162:VAL:HG23	2.14	0.47
2:B:135:THR:HG22	2:B:140:LEU:HD21	1.95	0.47
2:F:142:LEU:O	2:F:145:VAL:HG12	2.15	0.47
2:J:135:THR:O	2:J:135:THR:OG1	2.33	0.47
2:F:248:TRP:O	2:F:251:THR:OG1	2.28	0.47
1:G:22:ARG:HE	2:H:75:GLU:CD	2.22	0.47
1:G:22:ARG:HD3	1:G:72:LEU:HD21	1.97	0.47
1:K:26:ILE:HD11	2:L:75:GLU:HG2	1.97	0.47
2:D:218:ILE:HD13	2:D:253:VAL:HG23	1.96	0.47
1:K:24:ARG:NH1	1:K:31:LEU:O	2.44	0.46
2:L:158:LEU:HB3	2:L:280:MET:SD	2.55	0.46
2:D:227:HIS:HD1	2:D:228:TYR:H	1.62	0.46
1:E:56:GLY:O	1:E:93:SER:HB2	2.15	0.46
2:F:201:ARG:NE	2:F:292:GLU:OE2	2.46	0.46
2:L:216:TYR:CD1	2:L:255:VAL:HG22	2.50	0.46
1:A:123:THR:O	1:A:123:THR:HG22	2.15	0.46
2:B:207:ASP:HB3	2:B:210:TYR:O	2.16	0.46
2:D:137:ARG:HA	2:D:140:LEU:HD12	1.97	0.46
2:J:291:LEU:HD21	2:J:295:ARG:HH21	1.81	0.46
1:I:23:ILE:O	1:I:27:VAL:HG23	2.14	0.46
1:A:170:GLY:HA3	2:B:86:LEU:HD21	1.98	0.46
2:B:135:THR:HB	2:B:233:ARG:HG3	1.98	0.46
2:H:151:ILE:HG21	2:H:283:ILE:HD13	1.98	0.46
2:L:255:VAL:HG21	2:L:306:PRO:HD2	1.97	0.46
1:E:90:THR:OG1	1:E:93:SER:O	2.25	0.46
1:I:17:GLU:O	1:I:21:GLN:HG3	2.16	0.46
1:K:22:ARG:NH1	2:L:69:ALA:HB2	2.30	0.46
2:L:217:VAL:HB	2:L:254:LEU:HB3	1.98	0.46
1:K:41:TYR:CE2	1:K:47:PRO:HB3	2.51	0.46
2:H:260:ALA:O	2:H:263:PRO:HD3	2.16	0.45
2:J:162:VAL:HA	2:J:172:LEU:HD21	1.97	0.45
1:C:52:PHE:CE2	1:C:73:MET:HE3	2.51	0.45
2:F:111:GLY:O	1:I:90:THR:HG21	2.17	0.45
1:K:38:ALA:HB1	1:K:47:PRO:HG3	1.98	0.45
1:A:19:LEU:HD13	1:A:76:TRP:HB2	1.99	0.45
1:G:163:GLN:HB3	2:H:102:VAL:HG12	1.98	0.45
1:A:123:THR:HG21	2:J:94:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ARG:O	1:E:55:HIS:ND1	2.50	0.45
2:L:151:ILE:HD11	2:L:280:MET:HG3	1.99	0.45
2:L:215:LEU:HG	2:L:256:VAL:HB	1.99	0.45
2:B:192:LEU:HD13	2:B:217:VAL:HG11	1.99	0.45
2:J:164:LEU:HD13	2:J:297:TYR:CZ	2.52	0.45
2:D:191:ILE:HG21	2:D:234:MET:HG3	1.99	0.45
1:E:88:GLN:HG2	1:E:90:THR:H	1.82	0.45
2:H:201:ARG:HB2	2:H:218:ILE:HB	1.98	0.45
2:F:227:HIS:HB3	2:F:230:LEU:HB2	1.98	0.45
2:H:163:VAL:HG11	2:H:293:TYR:HB3	1.99	0.45
1:K:113:PRO:HD3	1:K:136:ILE:HG12	1.99	0.45
2:L:202:LEU:HD23	2:L:217:VAL:HA	1.99	0.45
1:A:111:ILE:HD13	1:A:128:LEU:HD22	1.99	0.45
1:E:25:LEU:HA	1:E:25:LEU:HD23	1.85	0.44
1:K:85:LEU:HD23	1:K:87:ILE:HD11	1.98	0.44
2:F:109:LEU:HD22	2:F:114:TYR:CD2	2.52	0.44
2:H:141:ILE:HG12	2:H:268:ILE:HG12	1.98	0.44
1:C:26:ILE:HD12	2:D:79:VAL:HG21	1.98	0.44
2:J:141:ILE:O	2:J:145:VAL:HG22	2.17	0.44
1:E:89:ASN:HB2	1:E:120:LEU:HB3	2.00	0.44
1:I:103:PRO:C	1:I:105:ASN:N	2.76	0.44
2:L:180:LEU:HD13	2:L:271:VAL:HG23	1.98	0.44
2:H:140:LEU:HD13	2:H:187:PHE:HB3	2.00	0.44
1:I:46:LEU:HG	1:I:100:PHE:CZ	2.53	0.44
1:I:153:ILE:HG12	1:I:166:PHE:CD1	2.52	0.44
2:H:163:VAL:O	2:H:167:ARG:HG2	2.18	0.44
1:G:24:ARG:NH2	1:G:28:PRO:O	2.46	0.44
2:H:203:LEU:O	2:H:215:LEU:HD12	2.18	0.44
1:C:159:MET:HB3	1:C:160:PRO:HD3	1.99	0.43
2:L:209:THR:HG22	2:L:210:TYR:CD1	2.53	0.43
2:L:68:LEU:HD13	2:L:75:GLU:HG3	2.00	0.43
2:L:247:VAL:HG12	2:L:252:PHE:CD1	2.54	0.43
1:C:146:PRO:HG3	2:D:61:TYR:CE1	2.54	0.43
2:D:204:PHE:CE1	2:D:215:LEU:HD13	2.53	0.43
2:J:192:LEU:HD13	2:J:217:VAL:HG11	1.99	0.43
2:J:227:HIS:CD2	2:J:229:LEU:HB2	2.53	0.43
2:H:107:LEU:HA	2:H:116:LEU:HD23	2.00	0.43
1:A:170:GLY:C	2:B:82:LEU:HD23	2.42	0.43
2:F:108:THR:HG22	2:F:225:HIS:HD2	1.83	0.43
1:I:112:THR:OG1	1:I:115:ARG:HB2	2.18	0.43
1:K:165:ALA:HB2	2:L:102:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:92:VAL:HG21	2:L:116:LEU:HG	2.00	0.43
1:C:22:ARG:O	1:C:26:ILE:HG12	2.19	0.43
2:F:88:LYS:HA	2:F:118:ILE:HD12	1.99	0.43
2:H:226:LEU:HB3	2:H:231:ILE:HD11	2.00	0.43
2:D:174:ASP:OD1	2:D:174:ASP:N	2.51	0.43
1:E:87:ILE:HG12	1:E:96:PHE:HD1	1.83	0.43
2:F:77:ALA:O	2:F:81:SER:OG	2.32	0.43
1:K:145:ARG:HB2	1:K:148:MET:HG3	2.00	0.43
2:F:146:GLN:HG2	2:F:149:ASN:HD21	1.83	0.43
2:H:94:LEU:HD21	2:H:109:LEU:HD21	1.99	0.43
2:J:137:ARG:O	2:J:141:ILE:HG13	2.18	0.43
2:L:216:TYR:HD1	2:L:255:VAL:HG22	1.83	0.43
1:A:173:ASP:OD1	1:A:174:ALA:N	2.51	0.43
1:G:27:VAL:HG11	1:G:54:PHE:CE2	2.54	0.43
2:B:111:GLY:O	1:K:90:THR:HG21	2.19	0.43
2:B:114:TYR:CZ	1:K:90:THR:O	2.72	0.43
2:D:182:GLN:NE2	2:D:213:HIS:O	2.45	0.43
1:E:51:ALA:N	1:E:98:GLY:O	2.40	0.43
2:H:216:TYR:CE1	2:H:255:VAL:HG23	2.54	0.43
2:J:218:ILE:HD13	2:J:253:VAL:HG23	2.01	0.43
1:A:16:PHE:HB2	1:A:41:TYR:CZ	2.54	0.42
1:A:111:ILE:HG22	1:A:111:ILE:O	2.18	0.42
2:B:98:LEU:HD11	2:B:254:LEU:HD11	1.99	0.42
1:C:75:ASP:OD1	2:D:62:ARG:HG3	2.19	0.42
1:C:86:ARG:NH1	1:C:97:GLN:OE1	2.53	0.42
1:E:70:LEU:HD22	1:E:83:PRO:HB2	2.01	0.42
1:E:137:LYS:HE3	1:E:149:ALA:HB3	2.01	0.42
2:H:106:CYS:SG	2:H:122:CYS:HB2	2.59	0.42
2:H:141:ILE:O	2:H:145:VAL:HG23	2.20	0.42
1:K:89:ASN:ND2	1:K:162:VAL:HG23	2.34	0.42
2:B:94:LEU:HD11	2:B:109:LEU:CD2	2.49	0.42
2:B:218:ILE:HD13	2:B:253:VAL:HG23	2.01	0.42
1:E:25:LEU:HD22	2:F:76:ILE:HD11	2.01	0.42
2:H:129:ASP:OD1	2:H:129:ASP:N	2.52	0.42
1:I:86:ARG:HH21	1:I:125:THR:HG21	1.84	0.42
1:I:89:ASN:O	1:I:91:GLY:N	2.48	0.42
1:G:132:ASP:O	1:G:136:ILE:HG12	2.20	0.42
1:I:27:VAL:HG21	1:I:54:PHE:CE2	2.54	0.42
2:J:94:LEU:HD12	2:J:114:TYR:CE2	2.54	0.42
1:K:41:TYR:CD2	1:K:47:PRO:HB3	2.55	0.42
2:L:184:GLU:HA	2:L:187:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:CYS:HB3	2:D:125:CYS:HB2	2.01	0.42
2:L:118:ILE:H	2:L:118:ILE:HG13	1.73	0.42
1:A:157:VAL:HG13	1:A:162:VAL:HG22	2.01	0.42
2:D:141:ILE:O	2:D:145:VAL:HG23	2.20	0.42
1:I:90:THR:HB	1:I:93:SER:O	2.20	0.42
1:I:22:ARG:HD3	1:I:72:LEU:HD21	2.01	0.42
1:I:22:ARG:NH2	2:J:65:PHE:O	2.42	0.42
1:A:24:ARG:HD2	1:A:54:PHE:HE1	1.85	0.41
2:B:74:GLU:O	2:B:78:ILE:HG13	2.20	0.41
1:I:128:LEU:HD11	1:I:132:ASP:HB2	2.02	0.41
2:B:217:VAL:HB	2:B:254:LEU:HB3	2.02	0.41
1:G:102:ARG:C	1:G:104:HIS:H	2.29	0.41
1:I:84:TYR:OH	1:I:127:GLY:HA3	2.20	0.41
2:D:68:LEU:HD23	2:D:68:LEU:HA	1.86	0.41
2:B:107:LEU:HA	2:B:116:LEU:HD23	2.01	0.41
1:C:17:GLU:O	1:C:20:VAL:HG12	2.20	0.41
1:C:120:LEU:HD11	1:C:126:THR:HG22	2.02	0.41
2:D:216:TYR:HE1	2:D:255:VAL:HG13	1.86	0.41
2:F:156:ALA:HB1	2:F:293:TYR:OH	2.21	0.41
1:G:50:CYS:SG	1:G:53:GLN:HG3	2.61	0.41
2:L:55:LEU:O	2:L:59:GLN:HG3	2.20	0.41
1:C:75:ASP:CG	2:D:62:ARG:HG3	2.45	0.41
2:D:54:CYS:O	2:D:58:ARG:NE	2.46	0.41
2:F:192:LEU:HB3	2:F:200:PRO:HG3	2.02	0.41
1:I:84:TYR:HE1	1:I:86:ARG:HB2	1.85	0.41
2:L:231:ILE:O	2:L:235:LEU:HG	2.21	0.41
1:C:110:ALA:HB2	1:C:166:PHE:CD2	2.56	0.41
1:E:86:ARG:NH1	1:E:97:GLN:OE1	2.53	0.41
2:F:107:LEU:HD23	2:F:226:LEU:HD12	2.01	0.41
1:A:75:ASP:OD2	2:B:62:ARG:HA	2.21	0.41
2:D:262:LYS:HB2	2:D:262:LYS:HE3	1.78	0.41
1:E:63:SER:HB3	1:E:152:TRP:CE3	2.56	0.41
1:E:84:TYR:OH	1:E:127:GLY:HA3	2.21	0.41
2:J:153:GLU:O	2:J:193:ARG:NH1	2.54	0.41
1:A:111:ILE:HD12	1:A:128:LEU:HB2	2.03	0.41
1:C:33:GLY:HA3	1:C:54:PHE:HA	2.02	0.41
1:C:66:ILE:HD12	1:C:85:LEU:HD23	2.03	0.41
2:D:162:VAL:HA	2:D:172:LEU:HD13	2.03	0.41
1:G:145:ARG:HB2	1:G:148:MET:HG3	2.03	0.41
2:L:158:LEU:O	2:L:162:VAL:HG23	2.21	0.41
2:D:164:LEU:HG	2:D:168:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:LEU:HD21	2:D:276:ILE:HB	2.02	0.41
1:I:25:LEU:HD23	1:I:25:LEU:HA	1.89	0.41
2:J:96:PHE:CZ	2:J:116:LEU:HD11	2.56	0.41
1:K:25:LEU:HB3	2:L:76:ILE:HD11	2.01	0.41
1:I:111:ILE:HG13	1:I:136:ILE:HD13	2.03	0.40
1:K:112:THR:O	1:K:115:ARG:HB3	2.21	0.40
2:F:218:ILE:HD13	2:F:253:VAL:HG23	2.04	0.40
1:I:170:GLY:HA3	2:J:86:LEU:HD21	2.04	0.40
2:J:196:GLY:O	2:J:199:ASP:N	2.55	0.40
1:K:19:LEU:HD11	1:K:72:LEU:HG	2.02	0.40
2:B:136:SER:O	2:B:140:LEU:HG	2.21	0.40
2:D:172:LEU:HD21	2:D:280:MET:HE2	2.03	0.40
1:E:163:GLN:HB3	2:F:102:VAL:HG13	2.03	0.40
2:H:157:PHE:O	2:H:161:LEU:HG	2.21	0.40
2:J:102:VAL:HG22	2:J:105:ASN:OD1	2.21	0.40
2:L:94:LEU:HA	2:L:95:PRO:C	2.46	0.40
2:B:163:VAL:HG23	2:B:290:MET:HE3	2.04	0.40
1:C:30:THR:HB	1:C:62:GLU:HG3	2.04	0.40
1:C:70:LEU:HD22	1:C:83:PRO:HB2	2.04	0.40
1:C:88:GLN:HG2	1:C:90:THR:HG23	2.04	0.40
2:F:94:LEU:HG	2:F:95:PRO:HA	2.04	0.40
2:F:94:LEU:HD21	2:F:246:HIS:C	2.46	0.40
2:F:201:ARG:HB2	2:F:218:ILE:HB	2.04	0.40
2:F:203:LEU:O	2:F:215:LEU:HD12	2.21	0.40
2:H:140:LEU:HB3	2:H:187:PHE:CD1	2.55	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	163/183 (89%)	152 (93%)	11 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	163/183 (89%)	150 (92%)	11 (7%)	2 (1%)	10	41
1	E	163/183 (89%)	152 (93%)	9 (6%)	2 (1%)	10	41
1	G	161/183 (88%)	149 (92%)	12 (8%)	0	100	100
1	I	161/183 (88%)	149 (92%)	11 (7%)	1 (1%)	21	56
1	K	162/183 (88%)	152 (94%)	9 (6%)	1 (1%)	21	56
2	B	251/260 (96%)	236 (94%)	12 (5%)	3 (1%)	10	41
2	D	251/260 (96%)	239 (95%)	11 (4%)	1 (0%)	30	65
2	F	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	65
2	H	246/260 (95%)	232 (94%)	13 (5%)	1 (0%)	30	65
2	J	248/260 (95%)	228 (92%)	18 (7%)	2 (1%)	16	50
2	L	244/260 (94%)	232 (95%)	11 (4%)	1 (0%)	30	65
All	All	2464/2658 (93%)	2308 (94%)	141 (6%)	15 (1%)	21	56

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	261	GLU
2	F	197	ALA
1	I	104	HIS
2	D	198	CYS
2	L	261	GLU
2	J	267	GLU
1	K	90	THR
2	B	260	ALA
1	E	108	GLY
2	B	208	PRO
1	E	114	GLU
2	H	199	ASP
1	C	160	PRO
1	C	175	GLY
2	J	199	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	137/150 (91%)	137 (100%)	0	100	100
1	C	137/150 (91%)	137 (100%)	0	100	100
1	E	137/150 (91%)	137 (100%)	0	100	100
1	G	135/150 (90%)	135 (100%)	0	100	100
1	I	135/150 (90%)	135 (100%)	0	100	100
1	K	136/150 (91%)	136 (100%)	0	100	100
2	B	209/214 (98%)	209 (100%)	0	100	100
2	D	209/214 (98%)	209 (100%)	0	100	100
2	F	209/214 (98%)	209 (100%)	0	100	100
2	H	208/214 (97%)	208 (100%)	0	100	100
2	J	206/214 (96%)	206 (100%)	0	100	100
2	L	206/214 (96%)	206 (100%)	0	100	100
All	All	2064/2184 (94%)	2064 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	C	57	HIS
1	C	101	HIS
2	D	56	HIS
2	D	146	GLN
2	D	168	HIS
1	E	101	HIS
2	F	173	GLN
1	G	53	GLN
2	H	246	HIS
1	I	21	GLN
1	I	53	GLN
2	J	259	ASN
1	K	117	ASN
2	L	149	ASN
2	L	189	HIS

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	165/183 (90%)	1.18	18 (10%)	10 13	41, 62, 89, 107	0
1	C	165/183 (90%)	1.15	18 (10%)	10 13	42, 63, 94, 118	0
1	E	165/183 (90%)	1.13	16 (9%)	13 15	43, 63, 93, 115	0
1	G	163/183 (89%)	1.21	18 (11%)	10 13	40, 66, 95, 111	0
1	I	163/183 (89%)	1.25	22 (13%)	7 10	41, 61, 93, 112	0
1	K	164/183 (89%)	1.09	13 (7%)	18 18	40, 63, 92, 110	0
2	B	253/260 (97%)	1.11	24 (9%)	14 15	39, 65, 107, 126	0
2	D	253/260 (97%)	1.13	32 (12%)	8 11	44, 70, 104, 124	0
2	F	253/260 (97%)	1.08	22 (8%)	16 16	44, 70, 106, 128	0
2	H	250/260 (96%)	1.05	20 (8%)	18 18	44, 70, 104, 116	0
2	J	250/260 (96%)	1.11	25 (10%)	12 14	40, 73, 110, 125	0
2	L	248/260 (95%)	1.05	25 (10%)	12 14	46, 73, 104, 124	0
All	All	2492/2658 (93%)	1.12	253 (10%)	12 14	39, 67, 103, 128	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	147	MET	5.1
2	F	260	ALA	4.1
1	I	100	PHE	3.8
2	D	147	GLN	3.7
2	L	68	LEU	3.6
1	I	35	ASP	3.6
2	D	135	THR	3.5
2	D	192	LEU	3.5
2	L	104	ASP	3.4
2	H	291	LEU	3.4
1	E	78	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	270	THR	3.4
1	C	57	HIS	3.4
1	I	123	THR	3.3
1	I	38	ALA	3.3
2	F	138	GLU	3.3
2	B	157	PHE	3.2
2	D	103	ALA	3.2
1	E	147	MET	3.2
2	J	172	LEU	3.2
1	C	39	GLY	3.2
2	J	111	GLY	3.1
1	C	119	ILE	3.1
2	D	251	THR	3.1
2	H	253	VAL	3.1
2	D	146	GLN	3.1
2	J	192	LEU	3.1
1	I	106	ALA	3.0
1	A	147	MET	3.0
1	E	111	ILE	3.0
1	A	32	ARG	3.0
2	H	157	PHE	3.0
1	G	150	SER	3.0
2	H	213	HIS	2.9
2	B	261	GLU	2.9
1	K	48	SER	2.9
1	A	132	ASP	2.9
2	B	79	VAL	2.9
2	F	264	THR	2.9
2	H	161	LEU	2.9
1	A	138	GLY	2.9
1	G	23	ILE	2.9
1	G	48	SER	2.9
2	J	135	THR	2.9
1	I	136	ILE	2.9
2	J	77	ALA	2.9
1	I	50	CYS	2.9
2	J	251	THR	2.8
2	D	261	GLU	2.8
2	H	260	ALA	2.8
2	L	103	ALA	2.8
2	F	148	ILE	2.8
2	B	75	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	302	GLU	2.8
1	A	92	VAL	2.8
1	C	147	MET	2.8
2	B	134	ALA	2.8
2	J	268	ILE	2.7
1	A	81	CYS	2.7
1	G	40	PRO	2.7
2	D	79	VAL	2.7
2	D	269	PRO	2.7
2	H	152	PHE	2.7
2	B	213	HIS	2.7
2	B	209	THR	2.7
1	E	173	ASP	2.7
1	I	16	PHE	2.7
2	J	79	VAL	2.7
2	B	114	TYR	2.7
2	H	290	MET	2.7
1	K	57	HIS	2.7
2	H	90	THR	2.7
1	K	81	CYS	2.7
1	I	140	LEU	2.7
1	C	107	PRO	2.6
2	L	146	GLN	2.6
1	I	90	THR	2.6
2	L	222	THR	2.6
1	C	37	GLU	2.6
1	E	92	VAL	2.6
1	G	34	GLY	2.6
2	F	124	ALA	2.6
2	D	290	MET	2.6
1	I	57	HIS	2.6
2	D	84	VAL	2.6
2	J	152	PHE	2.6
1	G	79	VAL	2.6
1	A	52	PHE	2.6
1	C	111	ILE	2.5
2	D	61	TYR	2.5
1	K	32	ARG	2.5
1	G	92	VAL	2.5
2	J	275	ASP	2.5
1	G	68	TYR	2.5
2	L	278	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	46	LEU	2.5
1	G	173	ASP	2.5
2	J	58	ARG	2.5
1	C	150	SER	2.5
1	I	114	GLU	2.5
2	H	64	LEU	2.5
2	F	129	ASP	2.5
2	J	220	PRO	2.5
2	B	135	THR	2.5
1	A	66	ILE	2.5
2	F	114	TYR	2.5
2	F	134	ALA	2.5
1	E	32	ARG	2.5
2	B	121	CYS	2.5
2	D	109	LEU	2.5
1	E	122	SER	2.5
2	L	115	TYR	2.5
2	D	279	LYS	2.4
2	D	104	ASP	2.4
1	A	135	THR	2.4
2	D	114	TYR	2.4
2	H	170	ALA	2.4
1	G	147	MET	2.4
1	A	68	TYR	2.4
2	F	57	GLU	2.4
2	J	171	PRO	2.4
2	F	87	VAL	2.4
1	E	87	ILE	2.4
1	E	81	CYS	2.4
2	L	54	CYS	2.4
2	B	266	ALA	2.4
2	J	133	ALA	2.4
1	A	160	PRO	2.4
2	B	101	THR	2.4
2	B	61	TYR	2.4
2	L	97	CYS	2.4
1	C	89	ASN	2.4
1	G	113	PRO	2.4
1	E	31	LEU	2.4
2	D	151	ILE	2.4
2	D	286	ASP	2.4
2	L	155	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	147	MET	2.4
1	C	78	GLU	2.4
1	K	174	ALA	2.4
2	H	232	ASP	2.3
1	I	77	ALA	2.3
2	B	154	HIS	2.3
1	A	91	GLY	2.3
1	G	76	TRP	2.3
2	L	121	CYS	2.3
1	E	148	MET	2.3
2	J	134	ALA	2.3
1	C	128	LEU	2.3
2	H	175	LEU	2.3
2	B	72	PRO	2.3
2	J	155	ARG	2.3
1	A	142	LEU	2.3
1	I	111	ILE	2.3
2	J	132	PHE	2.3
2	L	143	ALA	2.3
2	D	83	SER	2.3
1	I	98	GLY	2.3
2	D	130	GLY	2.3
2	J	253	VAL	2.3
2	B	264	THR	2.3
2	J	226	LEU	2.3
2	L	230	LEU	2.3
1	K	51	ALA	2.3
1	C	114	GLU	2.3
2	H	261	GLU	2.3
1	A	40	PRO	2.3
1	K	83	PRO	2.3
2	B	263	PRO	2.3
2	D	287	GLY	2.3
2	D	58	ARG	2.3
2	D	245	ALA	2.2
2	F	237	ALA	2.2
2	H	57	GLU	2.2
2	D	226	LEU	2.2
2	J	121	CYS	2.2
2	B	190	THR	2.2
1	A	173	ASP	2.2
1	G	35	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	237	ALA	2.2
1	C	68	TYR	2.2
2	D	110	SER	2.2
2	D	63	GLY	2.2
2	L	90	THR	2.2
2	B	199	ASP	2.2
2	D	246	HIS	2.2
1	C	164	LEU	2.2
2	H	219	PHE	2.2
2	L	285	PHE	2.2
2	J	97	CYS	2.2
2	B	230	LEU	2.2
2	F	64	LEU	2.2
2	L	295	ARG	2.2
2	D	148	ILE	2.2
1	I	62	GLU	2.2
2	L	236	THR	2.2
1	K	89	ASN	2.2
1	A	46	LEU	2.2
2	F	121	CYS	2.1
2	J	246	HIS	2.1
1	A	27	VAL	2.1
1	C	66	ILE	2.1
2	D	195	GLY	2.1
1	K	17	GLU	2.1
2	F	269	PRO	2.1
2	B	227	HIS	2.1
1	I	107	PRO	2.1
2	D	206	PRO	2.1
2	B	71	THR	2.1
1	G	38	ALA	2.1
1	C	100	PHE	2.1
1	K	173	ASP	2.1
1	I	108	GLY	2.1
1	G	169	MET	2.1
1	E	51	ALA	2.1
2	D	134	ALA	2.1
2	F	133	ALA	2.1
1	C	157	VAL	2.1
2	F	192	LEU	2.1
2	F	275	ASP	2.1
2	H	181	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	80	PRO	2.1
2	L	198	CYS	2.1
2	H	148	ILE	2.1
2	J	151	ILE	2.1
2	L	266	ALA	2.1
2	L	105	ASN	2.1
1	I	142	LEU	2.1
2	D	213	HIS	2.1
2	L	189	HIS	2.1
2	L	280	MET	2.1
2	H	87	VAL	2.1
2	F	265	ASP	2.0
2	J	232	ASP	2.0
2	B	133	ALA	2.0
2	L	296	LEU	2.0
2	J	87	VAL	2.0
2	F	214	MET	2.0
1	G	138	GLY	2.0
2	F	240	GLY	2.0
1	C	137	LYS	2.0
1	I	125	THR	2.0
1	A	75	ASP	2.0
1	E	46	LEU	2.0
1	K	46	LEU	2.0
2	F	140	LEU	2.0
1	K	69	VAL	2.0
2	B	280	MET	2.0
2	H	54	CYS	2.0
1	G	47	PRO	2.0
1	I	135	THR	2.0
1	E	166	PHE	2.0
1	E	106	ALA	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(Å ²)	Q<0.9
3	ZN	F	401	1/1	0.94	0.15	100,100,100,100	0
3	ZN	H	401	1/1	0.95	0.19	198,198,198,198	0
3	ZN	B	401	1/1	0.96	0.06	74,74,74,74	0
3	ZN	D	401	1/1	0.98	0.10	121,121,121,121	0
3	ZN	L	401	1/1	0.98	0.14	159,159,159,159	0
3	ZN	J	401	1/1	0.99	0.10	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.