



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:01 PM UTC

PDB ID : 1TUE / pdb_00001tue
Title : The X-ray Structure of the Papillomavirus Helicase in Complex with its Molecular Matchmaker E2
Authors : Abbate, E.A.; Berger, J.M.; Botchan, M.R.
Deposited on : 2004-06-24
Resolution : 2.10 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

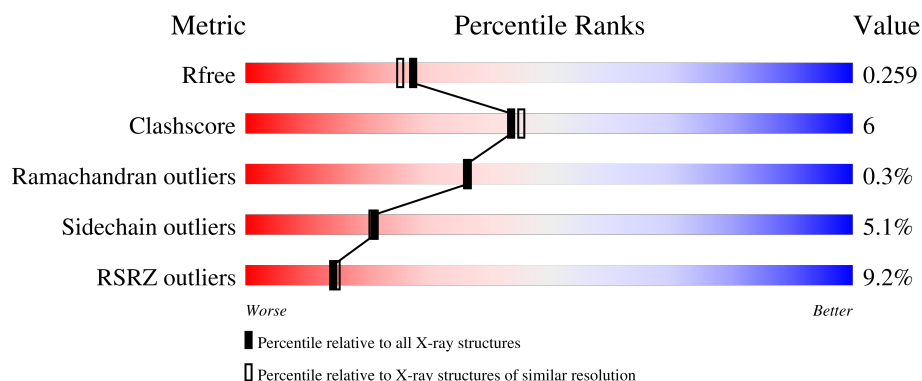
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	212	4% 76% 17% • 5%
1	D	212	3% 70% 22% • 5%
1	F	212	12% 75% 13% • 11%
1	H	212	4% 74% 16% 10%
1	K	212	3% 72% 18% 9%

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Mol	Chain	Length	Quality of chain
1	M	212	
2	B	218	
2	E	218	
2	G	218	
2	J	218	
2	L	218	
2	Q	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20186 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 Replication protein E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1645	1071	272	292	10			
1	D	202	Total	C	N	O	S	0	0	0
			1668	1087	280	291	10			
1	F	188	Total	C	N	O	S	0	0	0
			1551	1010	258	273	10			
1	H	191	Total	C	N	O	S	0	0	0
			1573	1025	261	277	10			
1	K	192	Total	C	N	O	S	0	0	0
			1584	1033	263	278	10			
1	M	196	Total	C	N	O	S	0	0	0
			1614	1054	266	284	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLY	-	expression tag	UNP P06789
A	421	SER	-	expression tag	UNP P06789
A	422	GLU	-	expression tag	UNP P06789
A	423	PHE	-	expression tag	UNP P06789
A	424	GLY	-	expression tag	UNP P06789
A	425	SER	-	expression tag	UNP P06789
A	426	GLY	-	expression tag	UNP P06789
A	427	SER	-	expression tag	UNP P06789
D	420	GLY	-	expression tag	UNP P06789
D	421	SER	-	expression tag	UNP P06789
D	422	GLU	-	expression tag	UNP P06789
D	423	PHE	-	expression tag	UNP P06789
D	424	GLY	-	expression tag	UNP P06789
D	425	SER	-	expression tag	UNP P06789
D	426	GLY	-	expression tag	UNP P06789
D	427	SER	-	expression tag	UNP P06789
F	420	GLY	-	expression tag	UNP P06789

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Chain	Residue	Modelled	Actual	Comment	Reference
F	421	SER	-	expression tag	UNP P06789
F	422	GLU	-	expression tag	UNP P06789
F	423	PHE	-	expression tag	UNP P06789
F	424	GLY	-	expression tag	UNP P06789
F	425	SER	-	expression tag	UNP P06789
F	426	GLY	-	expression tag	UNP P06789
F	427	SER	-	expression tag	UNP P06789
H	420	GLY	-	expression tag	UNP P06789
H	421	SER	-	expression tag	UNP P06789
H	422	GLU	-	expression tag	UNP P06789
H	423	PHE	-	expression tag	UNP P06789
H	424	GLY	-	expression tag	UNP P06789
H	425	SER	-	expression tag	UNP P06789
H	426	GLY	-	expression tag	UNP P06789
H	427	SER	-	expression tag	UNP P06789
K	420	GLY	-	expression tag	UNP P06789
K	421	SER	-	expression tag	UNP P06789
K	422	GLU	-	expression tag	UNP P06789
K	423	PHE	-	expression tag	UNP P06789
K	424	GLY	-	expression tag	UNP P06789
K	425	SER	-	expression tag	UNP P06789
K	426	GLY	-	expression tag	UNP P06789
K	427	SER	-	expression tag	UNP P06789
M	420	GLY	-	expression tag	UNP P06789
M	421	SER	-	expression tag	UNP P06789
M	422	GLU	-	expression tag	UNP P06789
M	423	PHE	-	expression tag	UNP P06789
M	424	GLY	-	expression tag	UNP P06789
M	425	SER	-	expression tag	UNP P06789
M	426	GLY	-	expression tag	UNP P06789
M	427	SER	-	expression tag	UNP P06789

- Molecule 2 is a protein called Regulatory protein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	0
			1599	1015	265	310	9			
2	E	196	Total	C	N	O	S	0	0	0
			1607	1020	266	313	8			
2	G	196	Total	C	N	O	S	0	0	0
			1608	1020	266	314	8			
2	J	194	Total	C	N	O	S	0	0	0
			1592	1010	264	310	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	193	Total	C	N	O	S	0	0	0
			1584	1006	262	308	8			
2	Q	194	Total	C	N	O	S	0	0	0
			1592	1010	264	310	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q80B71
B	-1	SER	-	expression tag	UNP Q80B71
B	0	HIS	-	expression tag	UNP Q80B71
E	-2	GLY	-	expression tag	UNP Q80B71
E	-1	SER	-	expression tag	UNP Q80B71
E	0	HIS	-	expression tag	UNP Q80B71
G	-2	GLY	-	expression tag	UNP Q80B71
G	-1	SER	-	expression tag	UNP Q80B71
G	0	HIS	-	expression tag	UNP Q80B71
J	-2	GLY	-	expression tag	UNP Q80B71
J	-1	SER	-	expression tag	UNP Q80B71
J	0	HIS	-	expression tag	UNP Q80B71
L	-2	GLY	-	expression tag	UNP Q80B71
L	-1	SER	-	expression tag	UNP Q80B71
L	0	HIS	-	expression tag	UNP Q80B71
Q	-2	GLY	-	expression tag	UNP Q80B71
Q	-1	SER	-	expression tag	UNP Q80B71
Q	0	HIS	-	expression tag	UNP Q80B71

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total	O	0	0
			132	132		
3	B	97	Total	O	0	0
			97	97		
3	D	109	Total	O	0	0
			109	109		
3	E	98	Total	O	0	0
			98	98		
3	F	67	Total	O	0	0
			67	67		
3	G	97	Total	O	0	0
			97	97		

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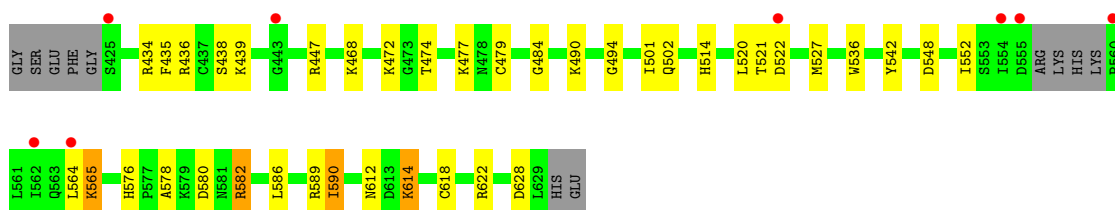
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	87	Total 87	O 87	0	0
3	J	54	Total 54	O 54	0	0
3	K	112	Total 112	O 112	0	0
3	L	32	Total 32	O 32	0	0
3	M	55	Total 55	O 55	0	0
3	Q	29	Total 29	O 29	0	0

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.

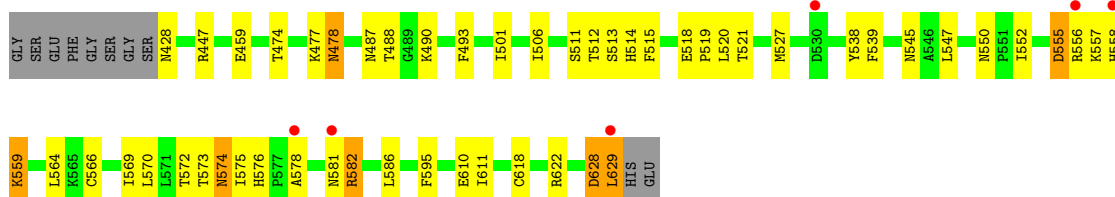
- Molecule 1: Replication protein E1

Chain A: 



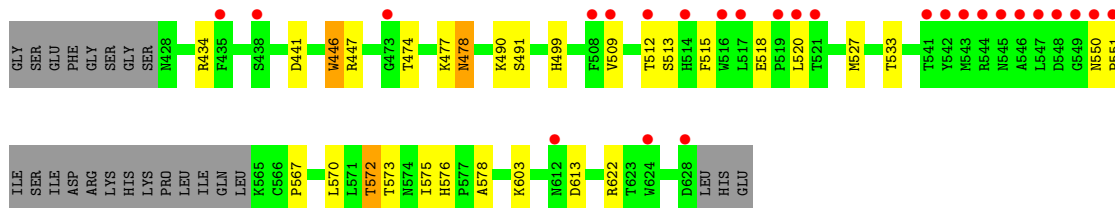
- Molecule 1: Replication protein E1

Chain D: 



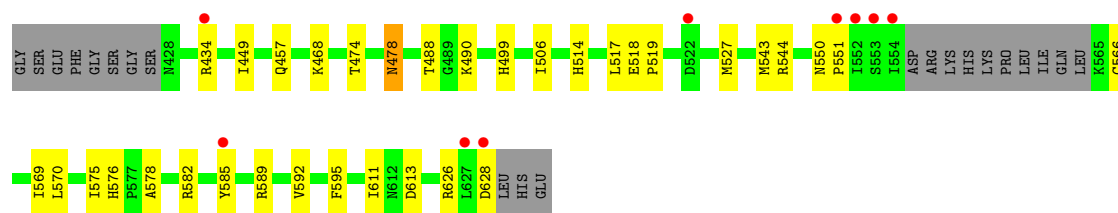
- Molecule 1: Replication protein E1

Chain F: 

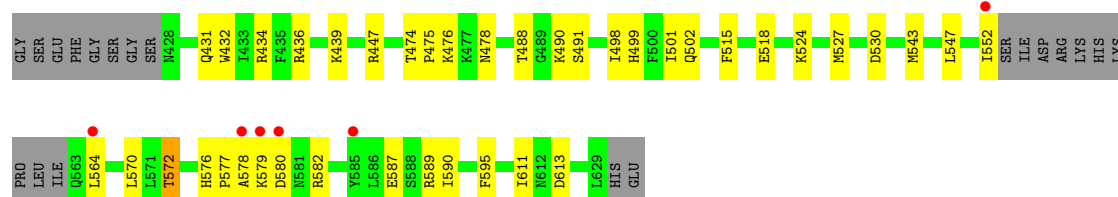
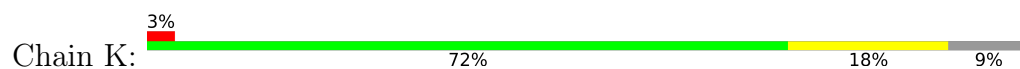


- Molecule 1: Replication protein E1

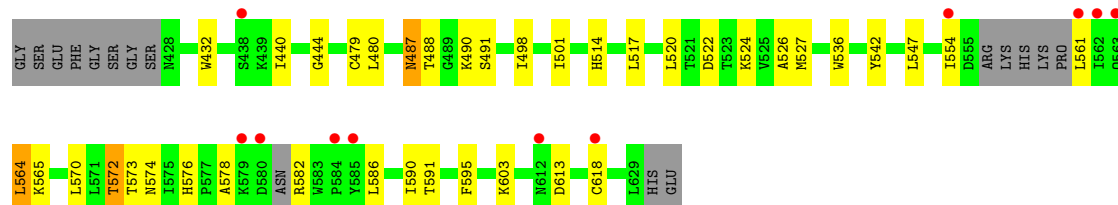
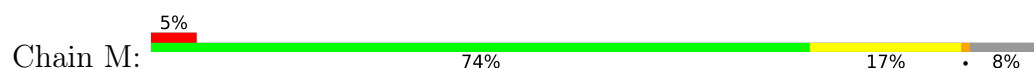
Chain H: 



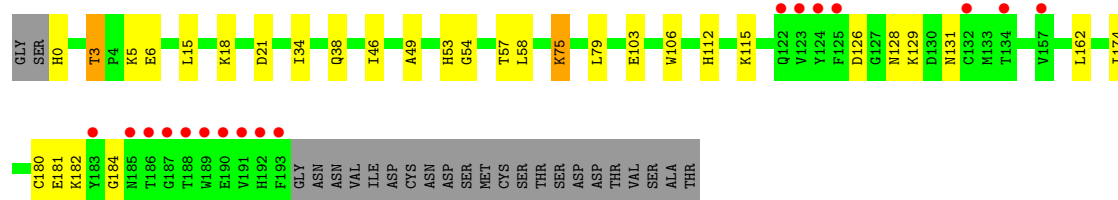
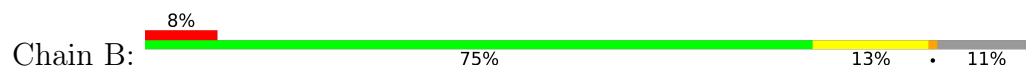
• Molecule 1: Replication protein E1



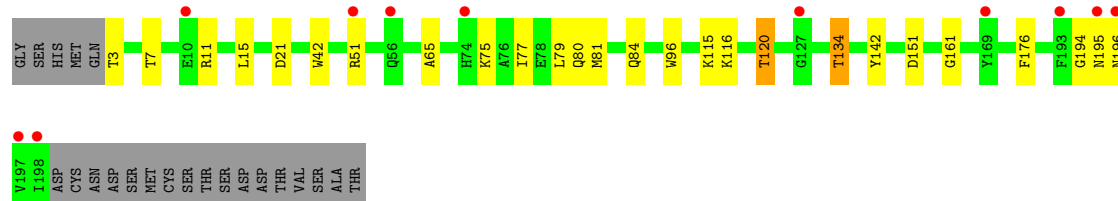
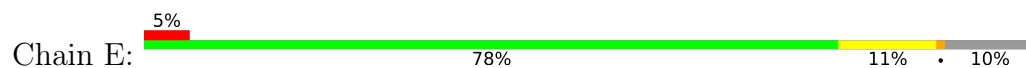
• Molecule 1: Replication protein E1



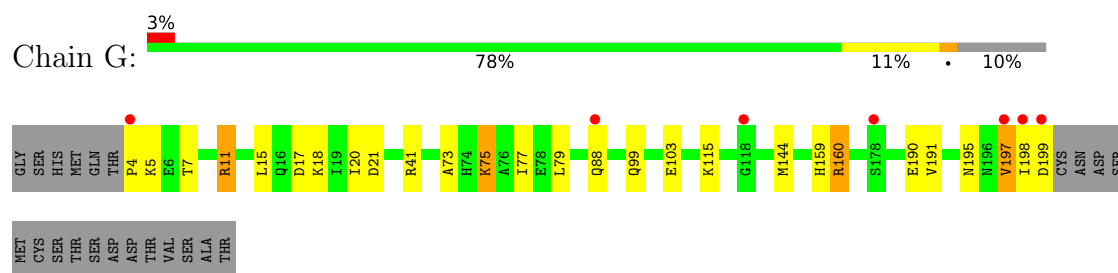
• Molecule 2: Regulatory protein E2



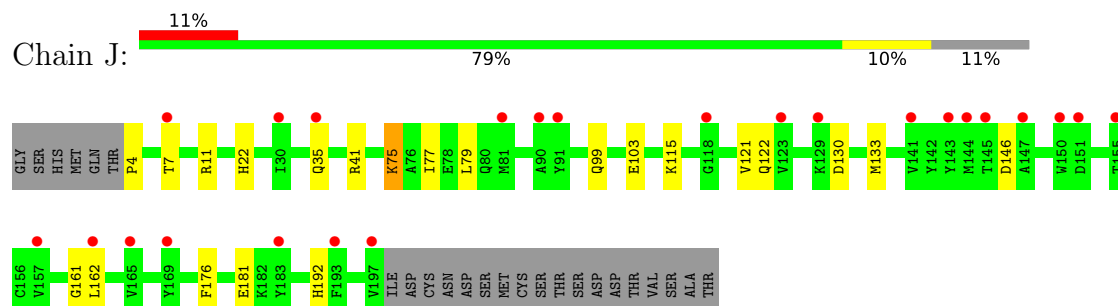
• Molecule 2: Regulatory protein E2



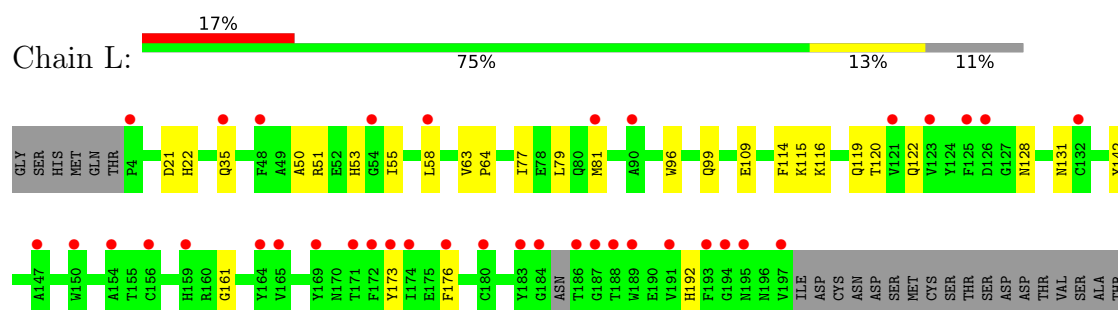
- Molecule 2: Regulatory protein E2



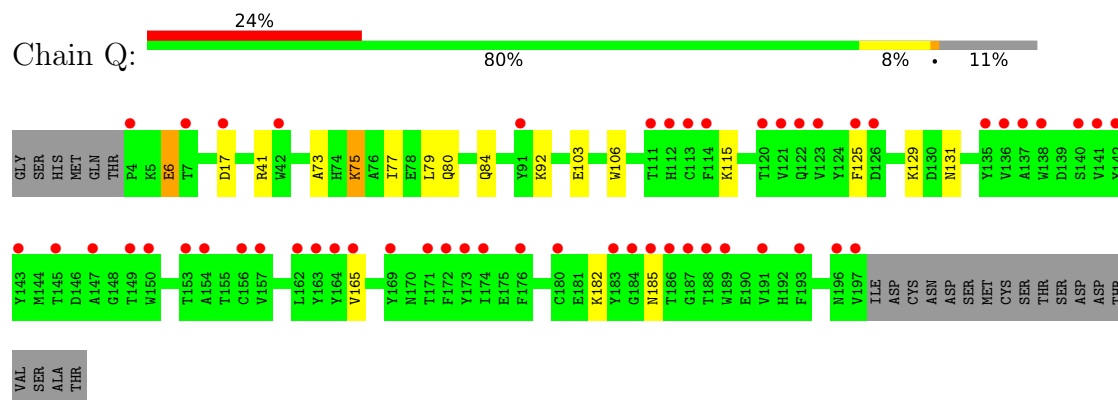
- Molecule 2: Regulatory protein E2



- Molecule 2: Regulatory protein E2



- Molecule 2: Regulatory protein E2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.30Å 88.75Å 375.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.10) 99.0 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.219 , 0.263 0.216 , 0.259	Depositor DCC
R_{free} test set	8003 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20186	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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](#)

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	0.57	0/1697	0.84	0/2304
1	D	0.53	0/1722	0.84	0/2338
1	F	0.48	0/1602	0.83	0/2175
1	H	0.52	0/1624	0.84	0/2205
1	K	0.52	0/1635	0.83	0/2220
1	M	0.48	0/1664	0.83	0/2258
2	B	0.50	0/1643	0.83	0/2229
2	E	0.50	0/1650	0.84	0/2240
2	G	0.47	0/1651	0.81	0/2240
2	J	0.45	0/1635	0.79	0/2218
2	L	0.44	0/1626	0.82	0/2204
2	Q	0.43	0/1635	0.80	0/2218
All	All	0.49	0/19784	0.83	0/26849

There are no bond length outliers.

There are no bond angle outliers.

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	1645	0	1599	24	0
1	D	1668	0	1632	35	0
1	F	1551	0	1495	17	0
1	H	1573	0	1522	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1584	0	1536	24	0
1	M	1614	0	1571	23	0
2	B	1599	0	1496	18	0
2	E	1607	0	1504	11	0
2	G	1608	0	1502	25	0
2	J	1592	0	1487	9	0
2	L	1584	0	1480	16	0
2	Q	1592	0	1487	8	0
3	A	132	0	0	2	0
3	B	97	0	0	0	0
3	D	109	0	0	7	0
3	E	98	0	0	0	0
3	F	67	0	0	0	0
3	G	97	0	0	4	0
3	H	87	0	0	1	0
3	J	54	0	0	2	0
3	K	112	0	0	5	0
3	L	32	0	0	1	0
3	M	55	0	0	0	0
3	Q	29	0	0	1	0
All	All	20186	0	18311	227	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 6.

All (227) 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:F:490:LYS:HE2	1:F:572:THR:HG23	1.32	1.11
2:G:159:HIS:HD2	2:G:198:ILE:CD1	1.65	1.08
2:L:55:ILE:HG21	2:L:58:LEU:HD21	1.41	1.02
1:M:520:LEU:CD2	1:M:526:ALA:HB2	1.91	1.00
1:H:518:GLU:HG3	1:H:519:PRO:HD3	1.44	0.97
2:G:159:HIS:CD2	2:G:198:ILE:CD1	2.47	0.96
2:G:159:HIS:CD2	2:G:198:ILE:HD11	2.01	0.95
1:M:520:LEU:CD2	1:M:526:ALA:CB	2.52	0.86
2:L:55:ILE:HG21	2:L:58:LEU:CD2	2.06	0.85
2:J:7:THR:O	2:J:11:ARG:HG2	1.78	0.84
1:K:576:HIS:HD2	1:K:578:ALA:H	1.23	0.84
2:G:191:VAL:H	2:G:198:ILE:HD12	1.44	0.80
2:Q:73:ALA:O	2:Q:77:ILE:HG13	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:520:LEU:HD21	1:M:526:ALA:CB	2.14	0.77
2:E:7:THR:O	2:E:11:ARG:HG2	1.84	0.76
2:B:49:ALA:O	2:B:53:HIS:HD2	1.69	0.75
2:G:159:HIS:HD2	2:G:198:ILE:CG1	2.00	0.75
1:M:490:LYS:HE2	1:M:572:THR:HG23	1.68	0.73
1:D:447:ARG:NH2	2:E:21:ASP:OD1	2.21	0.72
2:B:3:THR:HG22	2:B:6:GLU:H	1.54	0.72
1:D:582:ARG:HG3	1:D:582:ARG:HH11	1.54	0.71
1:F:576:HIS:HD2	1:F:578:ALA:H	1.38	0.71
2:B:75:LYS:HD2	2:B:103:GLU:HG3	1.73	0.70
1:F:491:SER:OG	1:F:572:THR:HG21	1.92	0.69
1:A:576:HIS:HD2	1:A:578:ALA:H	1.41	0.69
2:G:191:VAL:N	2:G:198:ILE:HD12	2.07	0.69
2:L:50:ALA:HB2	2:L:58:LEU:HD11	1.75	0.69
1:K:447:ARG:NH2	2:L:21:ASP:OD1	2.20	0.68
1:M:520:LEU:HD23	1:M:526:ALA:HB2	1.73	0.68
2:J:35:GLN:HB2	3:J:269:HOH:O	1.93	0.67
1:D:574:ASN:C	1:D:574:ASN:HD22	2.03	0.66
2:L:50:ALA:CB	2:L:58:LEU:HD11	2.27	0.65
2:G:159:HIS:HD2	2:G:198:ILE:HD11	1.42	0.65
2:Q:17:ASP:HB2	3:Q:226:HOH:O	1.96	0.65
1:H:576:HIS:HD2	1:H:578:ALA:H	1.44	0.65
1:A:447:ARG:NH2	2:B:21:ASP:OD1	2.29	0.65
1:H:518:GLU:HG3	1:H:519:PRO:CD	2.25	0.64
2:G:198:ILE:HG12	2:G:199:ASP:H	1.62	0.63
1:D:582:ARG:HG3	1:D:582:ARG:NH1	2.15	0.62
1:D:610:GLU:HA	3:D:727:HOH:O	1.99	0.62
1:F:474:THR:OG1	1:F:477:LYS:HB2	1.99	0.61
1:D:566:CYS:SG	1:D:569:ILE:HD11	2.40	0.61
1:K:491:SER:OG	1:K:572:THR:HG21	2.01	0.60
2:J:41:ARG:HD2	2:J:77:ILE:HG12	1.81	0.60
1:K:439:LYS:HE3	3:K:711:HOH:O	2.01	0.60
1:K:579:LYS:HE3	3:K:650:HOH:O	2.01	0.60
2:G:159:HIS:HD2	2:G:198:ILE:HG12	1.66	0.60
2:Q:75:LYS:HD2	2:Q:103:GLU:HG3	1.84	0.60
1:D:459:GLU:HG3	3:D:633:HOH:O	2.02	0.59
1:D:576:HIS:HD2	1:D:578:ALA:H	1.50	0.59
1:K:578:ALA:HA	1:K:587:GLU:HG2	1.85	0.59
1:H:517:LEU:C	1:H:519:PRO:HD2	2.28	0.58
2:B:3:THR:HG21	3:G:309:HOH:O	2.01	0.58
1:D:545:ASN:HD22	1:D:550:ASN:HD22	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:GLY:C	1:A:527:MET:HE1	2.27	0.58
1:D:556:ARG:HB2	1:D:559:LYS:HB2	1.85	0.58
1:K:431:GLN:NE2	3:K:741:HOH:O	2.36	0.58
1:A:514:HIS:HE1	1:A:542:TYR:O	1.87	0.57
1:D:581:ASN:HB3	3:D:696:HOH:O	2.02	0.57
2:G:159:HIS:CD2	2:G:198:ILE:HD13	2.35	0.57
1:M:520:LEU:HD22	1:M:526:ALA:HB2	1.85	0.57
2:B:15:LEU:HD12	2:B:46:ILE:HD12	1.86	0.57
1:K:530:ASP:H	1:K:572:THR:HG22	1.70	0.57
2:B:49:ALA:O	2:B:53:HIS:CD2	2.55	0.56
1:A:548:ASP:OD1	1:A:589:ARG:NH1	2.35	0.56
1:D:506:ILE:CG2	1:D:520:LEU:HD21	2.35	0.56
1:K:515:PHE:O	1:K:518:GLU:HB2	2.06	0.56
1:D:513:SER:C	1:D:515:PHE:H	2.14	0.56
1:K:499:HIS:HD2	1:K:613:ASP:OD1	1.87	0.55
2:B:180:CYS:C	2:B:182:LYS:H	2.14	0.55
1:F:520:LEU:HD22	1:F:567:PRO:HD2	1.88	0.55
2:B:34:ILE:O	2:B:38:GLN:HG3	2.06	0.55
2:G:7:THR:O	2:G:11:ARG:HG2	2.07	0.54
2:J:121:VAL:HG21	2:J:162:LEU:HD21	1.89	0.54
1:A:435:PHE:O	1:A:438:SER:HB2	2.07	0.54
1:F:478:ASN:HD22	1:F:478:ASN:H	1.56	0.54
1:H:506:ILE:HD12	1:H:519:PRO:HG2	1.90	0.54
1:A:434:ARG:NH2	3:A:671:HOH:O	2.41	0.54
1:A:614:LYS:NZ	1:A:614:LYS:HB3	2.21	0.54
1:A:580:ASP:OD1	1:A:582:ARG:HB2	2.09	0.53
1:D:521:THR:HA	1:D:564:LEU:HD13	1.90	0.53
1:D:618:CYS:O	1:D:622:ARG:HG3	2.08	0.53
1:K:498:ILE:HG13	1:K:527:MET:HB2	1.89	0.53
1:A:494:GLY:HA3	1:A:527:MET:HE1	1.89	0.53
1:D:490:LYS:HE2	1:D:572:THR:HB	1.91	0.53
1:M:432:TRP:CD1	1:M:524:LYS:HG3	2.43	0.53
2:G:159:HIS:CD2	2:G:198:ILE:HG12	2.44	0.53
2:G:144:MET:HE3	3:G:250:HOH:O	2.08	0.53
1:D:428:ASN:N	3:D:674:HOH:O	2.41	0.52
1:M:488:THR:HG21	1:M:595:PHE:O	2.09	0.52
2:L:22:HIS:HE1	2:L:35:GLN:NE2	2.07	0.52
1:A:580:ASP:OD2	1:A:582:ARG:NH2	2.38	0.52
1:A:472:LYS:NZ	1:A:628:ASP:HB3	2.25	0.51
2:L:109:GLU:HG3	2:L:173:TYR:HB2	1.92	0.51
1:F:490:LYS:CE	1:F:572:THR:HG23	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:LYS:HE3	1:D:573:THR:O	2.11	0.51
2:L:77:ILE:HG22	2:L:81:MET:HE2	1.93	0.51
1:M:491:SER:OG	1:M:572:THR:HG21	2.11	0.51
2:L:51:ARG:C	2:L:53:HIS:H	2.19	0.51
1:A:484:GLY:O	1:A:490:LYS:NZ	2.44	0.50
1:A:618:CYS:O	1:A:622:ARG:HG3	2.12	0.50
2:B:126:ASP:C	2:B:128:ASN:H	2.18	0.50
1:F:550:ASN:HB3	1:F:551:PRO:CD	2.42	0.50
1:M:576:HIS:HD2	1:M:578:ALA:H	1.58	0.50
2:G:73:ALA:O	2:G:77:ILE:HG13	2.12	0.50
2:G:41:ARG:NE	2:G:77:ILE:HG12	2.26	0.50
1:D:511:SER:O	1:D:538:TYR:HE1	1.95	0.50
1:A:436:ARG:NE	1:A:502:GLN:HG3	2.27	0.50
2:B:5:LYS:HE3	2:B:57:THR:O	2.12	0.50
1:D:574:ASN:HB2	3:D:728:HOH:O	2.12	0.49
1:K:490:LYS:HE2	1:K:572:THR:HG23	1.94	0.49
1:A:521:THR:HA	1:A:564:LEU:HD21	1.94	0.49
1:M:514:HIS:HB3	1:M:517:LEU:HD12	1.93	0.49
1:F:533:THR:HG22	1:F:575:ILE:HG21	1.95	0.49
2:J:75:LYS:HD2	2:J:103:GLU:HG3	1.93	0.49
2:E:51:ARG:HH21	2:E:65:ALA:HA	1.77	0.49
1:H:517:LEU:HD11	1:H:543:MET:SD	2.53	0.49
1:F:490:LYS:HE2	1:F:572:THR:CG2	2.23	0.49
1:H:544:ARG:HG2	1:H:589:ARG:HH12	1.77	0.48
1:M:487:ASN:C	1:M:487:ASN:HD22	2.21	0.48
1:D:539:PHE:HB3	1:D:586:LEU:HD21	1.95	0.48
2:G:199:ASP:HB2	3:G:310:HOH:O	2.12	0.48
1:A:565:LYS:HE2	3:A:752:HOH:O	2.13	0.48
1:D:628:ASP:O	1:D:629:LEU:HB2	2.11	0.48
1:F:499:HIS:HD2	1:F:613:ASP:OD1	1.97	0.48
1:K:436:ARG:CZ	1:K:502:GLN:HG3	2.44	0.48
1:F:527:MET:HA	1:F:570:LEU:O	2.14	0.47
1:M:554:ILE:HD11	1:M:564:LEU:HD22	1.95	0.47
2:G:191:VAL:HB	2:G:198:ILE:HG13	1.94	0.47
1:K:576:HIS:HB3	1:K:579:LYS:HE2	1.96	0.47
2:Q:41:ARG:HD2	2:Q:77:ILE:HG12	1.96	0.47
1:D:474:THR:HB	1:D:477:LYS:HB2	1.97	0.47
1:D:506:ILE:HG21	1:D:520:LEU:HD21	1.97	0.47
1:H:518:GLU:N	1:H:519:PRO:HD2	2.29	0.47
2:L:122:GLN:HB2	2:L:192:HIS:HB2	1.97	0.47
2:B:15:LEU:CD1	2:B:46:ILE:HD12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:434:ARG:NE	3:K:741:HOH:O	2.47	0.47
1:M:479:CYS:HB2	1:M:547:LEU:HD22	1.97	0.47
2:B:162:LEU:HD12	2:B:174:ILE:HG13	1.96	0.47
1:F:446:TRP:CD2	1:F:622:ARG:HD2	2.50	0.46
1:M:490:LYS:HE3	1:M:573:THR:O	2.15	0.46
1:A:468:LYS:HE3	1:A:628:ASP:HB2	1.97	0.46
1:A:479:CYS:HB2	1:A:590:ILE:HG22	1.98	0.46
1:A:612:ASN:OD1	1:A:614:LYS:HG2	2.15	0.46
1:D:518:GLU:N	1:D:519:PRO:HD2	2.30	0.46
2:G:88:GLN:OE1	1:H:582:ARG:NH1	2.46	0.46
2:B:75:LYS:HE2	2:B:106:TRP:HD1	1.80	0.46
1:D:545:ASN:ND2	1:D:550:ASN:HD22	2.14	0.46
2:J:161:GLY:HA2	2:J:176:PHE:CD1	2.50	0.46
2:E:80:GLN:O	2:E:84:GLN:HG3	2.15	0.46
1:H:506:ILE:CD1	1:H:519:PRO:HG2	2.46	0.45
2:J:122:GLN:HB2	2:J:192:HIS:HB2	1.97	0.45
1:D:511:SER:HB2	3:D:705:HOH:O	2.16	0.45
1:F:550:ASN:HB3	1:F:551:PRO:HD2	1.97	0.45
1:H:499:HIS:HD2	1:H:613:ASP:OD1	2.00	0.45
1:K:577:PRO:HG2	1:K:590:ILE:HD12	1.98	0.45
2:E:120:THR:HG23	2:E:134:THR:HG23	1.98	0.45
1:H:478:ASN:HD22	1:H:478:ASN:H	1.64	0.45
1:K:576:HIS:CD2	1:K:578:ALA:H	2.16	0.45
1:A:494:GLY:CA	1:A:527:MET:HE1	2.46	0.45
1:M:514:HIS:HE1	1:M:542:TYR:O	2.00	0.45
2:B:3:THR:CG2	2:B:6:GLU:H	2.25	0.45
1:K:476:LYS:HG2	1:K:589:ARG:HG2	1.98	0.45
2:E:161:GLY:HA2	2:E:176:PHE:CE1	2.52	0.45
2:E:77:ILE:O	2:E:81:MET:HG2	2.16	0.44
2:Q:6:GLU:H	2:Q:6:GLU:HG2	1.59	0.44
2:E:96:TRP:CZ3	2:E:116:LYS:HE3	2.52	0.44
1:H:514:HIS:ND1	1:H:517:LEU:HD12	2.33	0.44
2:B:0:HIS:HE1	2:B:6:GLU:OE1	2.00	0.44
2:G:4:PRO:N	3:G:271:HOH:O	2.50	0.44
2:E:161:GLY:HA2	2:E:176:PHE:CD1	2.52	0.44
1:A:522:ASP:OD1	1:A:522:ASP:N	2.49	0.44
1:F:509:VAL:HG11	1:F:515:PHE:CZ	2.53	0.44
1:K:527:MET:HA	1:K:570:LEU:O	2.18	0.44
1:D:513:SER:OG	1:D:515:PHE:HB3	2.18	0.44
1:M:444:GLY:C	1:M:618:CYS:SG	3.02	0.43
1:F:447:ARG:NH2	2:G:21:ASP:OD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:75:LYS:HG2	2:G:103:GLU:CD	2.44	0.43
1:H:468:LYS:HE2	1:H:626:ARG:O	2.19	0.43
2:L:63:VAL:HA	2:L:64:PRO:HD3	1.83	0.43
2:E:15:LEU:HD21	2:E:42:TRP:HE3	1.83	0.43
1:H:576:HIS:HD2	1:H:578:ALA:N	2.15	0.43
1:H:585:TYR:O	1:H:589:ARG:HG3	2.19	0.43
1:H:527:MET:HA	1:H:570:LEU:O	2.19	0.43
2:L:128:ASN:HD22	2:L:131:ASN:HB2	1.84	0.43
1:A:536:TRP:CE3	1:A:586:LEU:HD21	2.54	0.43
1:K:543:MET:O	1:K:547:LEU:HG	2.18	0.43
2:Q:80:GLN:HE21	2:Q:84:GLN:NE2	2.17	0.43
1:K:502:GLN:HG2	3:K:658:HOH:O	2.18	0.43
1:M:536:TRP:CE3	1:M:586:LEU:HD21	2.54	0.42
2:B:106:TRP:CZ2	2:B:112:HIS:HA	2.54	0.42
1:D:478:ASN:HD21	1:D:547:LEU:HA	1.84	0.42
1:M:527:MET:HA	1:M:570:LEU:O	2.19	0.42
2:J:22:HIS:CE1	2:J:35:GLN:HG2	2.55	0.42
2:E:142:TYR:HA	2:E:151:ASP:O	2.19	0.42
1:M:440:ILE:HD12	1:M:613:ASP:HB3	2.01	0.42
2:Q:75:LYS:HE2	2:Q:106:TRP:HD1	1.83	0.42
1:D:574:ASN:C	1:D:574:ASN:ND2	2.76	0.42
1:H:566:CYS:SG	1:H:569:ILE:HD11	2.60	0.42
2:J:4:PRO:HA	3:J:264:HOH:O	2.20	0.42
1:K:432:TRP:CD1	1:K:524:LYS:HG3	2.55	0.42
1:D:493:PHE:HD1	1:D:611:ILE:HD13	1.84	0.42
2:G:11:ARG:HG2	2:G:11:ARG:H	1.67	0.42
1:H:488:THR:HG21	1:H:595:PHE:O	2.19	0.42
1:H:576:HIS:CE1	1:H:592:VAL:HG11	2.55	0.42
1:M:498:ILE:HG13	1:M:527:MET:HB2	2.02	0.42
2:B:54:GLY:HA2	2:G:160:ARG:HH11	1.84	0.41
1:H:550:ASN:HA	1:H:551:PRO:HD3	1.92	0.41
2:L:114:PHE:HB2	2:L:142:TYR:HB2	2.02	0.41
2:L:96:TRP:CZ3	2:L:116:LYS:HE3	2.56	0.41
2:G:190:GLU:HA	2:G:198:ILE:HD12	2.02	0.41
2:L:22:HIS:HD2	3:L:229:HOH:O	2.03	0.41
2:L:161:GLY:HA2	2:L:176:PHE:CD1	2.55	0.41
1:F:490:LYS:HE3	1:F:573:THR:O	2.21	0.41
1:M:586:LEU:O	1:M:590:ILE:HG12	2.20	0.41
2:Q:125:PHE:HB2	2:Q:131:ASN:ND2	2.36	0.41
2:G:198:ILE:HG23	2:G:199:ASP:N	2.35	0.41
1:D:527:MET:HA	1:D:570:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:THR:HB	1:A:477:LYS:HB2	2.03	0.41
1:H:449:ILE:HG12	1:H:611:ILE:HG23	2.03	0.41
1:K:475:PRO:O	1:K:476:LYS:HB2	2.20	0.41
1:K:488:THR:HG21	1:K:595:PHE:O	2.21	0.41
1:D:513:SER:C	1:D:515:PHE:N	2.79	0.40
1:D:555:ASP:HB3	3:D:739:HOH:O	2.21	0.40
1:H:457:GLN:NE2	3:H:715:HOH:O	2.50	0.40
1:M:574:ASN:HD22	1:M:574:ASN:HA	1.73	0.40
1:D:488:THR:HG21	1:D:595:PHE:O	2.20	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	197/212 (93%)	194 (98%)	3 (2%)	0	100	100
1	D	200/212 (94%)	190 (95%)	8 (4%)	2 (1%)	12	9
1	F	184/212 (87%)	177 (96%)	7 (4%)	0	100	100
1	H	187/212 (88%)	181 (97%)	6 (3%)	0	100	100
1	K	188/212 (89%)	186 (99%)	2 (1%)	0	100	100
1	M	190/212 (90%)	187 (98%)	3 (2%)	0	100	100
2	B	192/218 (88%)	185 (96%)	5 (3%)	2 (1%)	12	9
2	E	194/218 (89%)	190 (98%)	3 (2%)	1 (0%)	24	22
2	G	194/218 (89%)	187 (96%)	6 (3%)	1 (0%)	24	22
2	J	192/218 (88%)	187 (97%)	5 (3%)	0	100	100
2	L	189/218 (87%)	180 (95%)	9 (5%)	0	100	100
2	Q	192/218 (88%)	186 (97%)	5 (3%)	1 (0%)	24	22
All	All	2299/2580 (89%)	2230 (97%)	62 (3%)	7 (0%)	36	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	184	GLY
2	E	194	GLY
2	G	197	VAL
2	Q	185	ASN
2	B	181	GLU
1	D	557	LYS
1	D	514	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/191 (95%)	174 (96%)	8 (4%)	25	26
1	D	184/191 (96%)	171 (93%)	13 (7%)	13	11
1	F	170/191 (89%)	161 (95%)	9 (5%)	20	19
1	H	173/191 (91%)	167 (96%)	6 (4%)	32	35
1	K	174/191 (91%)	165 (95%)	9 (5%)	21	20
1	M	178/191 (93%)	167 (94%)	11 (6%)	16	14
2	B	171/192 (89%)	163 (95%)	8 (5%)	23	24
2	E	172/192 (90%)	164 (95%)	8 (5%)	23	24
2	G	172/192 (90%)	159 (92%)	13 (8%)	12	9
2	J	170/192 (88%)	162 (95%)	8 (5%)	23	24
2	L	169/192 (88%)	164 (97%)	5 (3%)	36	41
2	Q	170/192 (88%)	162 (95%)	8 (5%)	23	24
All	All	2085/2298 (91%)	1979 (95%)	106 (5%)	21	21

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	LYS
1	A	501	ILE

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Mol	Chain	Res	Type
1	A	520	LEU
1	A	552	ILE
1	A	565	LYS
1	A	582	ARG
1	A	590	ILE
1	A	614	LYS
2	B	3	THR
2	B	18	LYS
2	B	58	LEU
2	B	75	LYS
2	B	79	LEU
2	B	115	LYS
2	B	129	LYS
2	B	131	ASN
1	D	478	ASN
1	D	487	ASN
1	D	501	ILE
1	D	512	THR
1	D	552	ILE
1	D	555	ASP
1	D	558	HIS
1	D	559	LYS
1	D	574	ASN
1	D	575	ILE
1	D	582	ARG
1	D	628	ASP
1	D	629	LEU
2	E	3	THR
2	E	75	LYS
2	E	79	LEU
2	E	115	LYS
2	E	120	THR
2	E	134	THR
2	E	195	ASN
2	E	196	ASN
1	F	434	ARG
1	F	441	ASP
1	F	446	TRP
1	F	478	ASN
1	F	512	THR
1	F	513	SER
1	F	518	GLU

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Mol	Chain	Res	Type
1	F	572	THR
1	F	603	LYS
2	G	5	LYS
2	G	11	ARG
2	G	15	LEU
2	G	17	ASP
2	G	18	LYS
2	G	20	ILE
2	G	75	LYS
2	G	79	LEU
2	G	99	GLN
2	G	115	LYS
2	G	160	ARG
2	G	195	ASN
2	G	197	VAL
1	H	434	ARG
1	H	474	THR
1	H	478	ASN
1	H	490	LYS
1	H	575	ILE
1	H	628	ASP
2	J	75	LYS
2	J	79	LEU
2	J	99	GLN
2	J	115	LYS
2	J	130	ASP
2	J	133	MET
2	J	146	ASP
2	J	181	GLU
1	K	474	THR
1	K	478	ASN
1	K	501	ILE
1	K	552	ILE
1	K	564	LEU
1	K	572	THR
1	K	580	ASP
1	K	582	ARG
1	K	611	ILE
2	L	79	LEU
2	L	99	GLN
2	L	115	LYS
2	L	119	GLN

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Mol	Chain	Res	Type
2	L	120	THR
1	M	480	LEU
1	M	487	ASN
1	M	501	ILE
1	M	522	ASP
1	M	561	LEU
1	M	564	LEU
1	M	565	LYS
1	M	572	THR
1	M	582	ARG
1	M	591	THR
1	M	603	LYS
2	Q	6	GLU
2	Q	75	LYS
2	Q	79	LEU
2	Q	92	LYS
2	Q	115	LYS
2	Q	129	LYS
2	Q	165	VAL
2	Q	182	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	502	GLN
1	A	510	ASN
1	A	514	HIS
1	A	576	HIS
1	A	581	ASN
1	A	604	ASN
2	B	0	HIS
2	B	2	GLN
2	B	35	GLN
2	B	53	HIS
2	B	84	GLN
1	D	478	ASN
1	D	487	ASN
1	D	514	HIS
1	D	545	ASN
1	D	563	GLN
1	D	574	ASN
1	D	576	HIS

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Mol	Chain	Res	Type
2	E	35	GLN
2	E	44	ASN
2	E	80	GLN
2	E	107	ASN
1	F	478	ASN
1	F	499	HIS
1	F	576	HIS
2	G	16	GLN
2	G	35	GLN
2	G	99	GLN
2	G	159	HIS
2	G	185	ASN
2	G	195	ASN
1	H	478	ASN
1	H	499	HIS
1	H	576	HIS
2	J	35	GLN
2	J	61	GLN
2	J	80	GLN
2	J	99	GLN
1	K	499	HIS
1	K	510	ASN
1	K	576	HIS
2	L	16	GLN
2	L	22	HIS
2	L	35	GLN
2	L	99	GLN
2	L	119	GLN
2	L	128	ASN
2	L	159	HIS
2	L	195	ASN
1	M	431	GLN
1	M	487	ASN
1	M	499	HIS
1	M	514	HIS
1	M	574	ASN
1	M	576	HIS
2	Q	84	GLN
2	Q	128	ASN
2	Q	131	ASN
2	Q	159	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](#)

There are no ligands in this entry.

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	201/212 (94%)	-0.02	8 (3%) 42 44	16, 25, 48, 68	0
1	D	202/212 (95%)	0.18	6 (2%) 52 55	20, 29, 44, 58	0
1	F	188/212 (88%)	0.89	26 (13%) 6 6	26, 42, 73, 96	0
1	H	191/212 (90%)	0.39	9 (4%) 36 38	20, 33, 53, 73	0
1	K	192/212 (90%)	0.30	6 (3%) 51 54	20, 33, 55, 62	0
1	M	196/212 (92%)	0.49	11 (5%) 30 32	30, 40, 56, 70	0
2	B	194/218 (88%)	0.43	17 (8%) 15 16	18, 32, 76, 83	0
2	E	196/218 (89%)	0.26	11 (5%) 30 32	21, 30, 49, 69	0
2	G	196/218 (89%)	0.40	7 (3%) 46 48	25, 36, 49, 71	0
2	J	194/218 (88%)	0.95	24 (12%) 8 8	26, 47, 67, 81	0
2	L	193/218 (88%)	1.24	37 (19%) 3 3	26, 52, 98, 101	0
2	Q	194/218 (88%)	1.40	53 (27%) 1 1	30, 60, 96, 101	0
All	All	2337/2580 (90%)	0.57	215 (9%) 14 15	16, 36, 75, 101	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	554	ILE	4.7
2	J	197	VAL	4.7
2	L	197	VAL	4.7
2	G	198	ILE	4.7
2	L	123	VAL	4.6
2	Q	123	VAL	4.5
2	L	186	THR	4.5
2	L	125	PHE	4.5
2	J	147	ALA	4.4
2	Q	173	TYR	4.4
2	Q	197	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	551	PRO	4.3
1	F	547	LEU	4.3
1	F	544	ARG	4.3
1	F	546	ALA	4.2
2	Q	150	TRP	4.1
2	Q	4	PRO	4.1
2	Q	193	PHE	4.1
2	G	197	VAL	4.0
1	A	560	PRO	4.0
2	L	191	VAL	4.0
1	F	542	TYR	4.0
2	L	183	TYR	4.0
1	A	555	ASP	3.9
2	L	4	PRO	3.9
1	F	512	THR	3.9
2	L	193	PHE	3.9
1	K	580	ASP	3.8
2	L	154	ALA	3.8
1	M	561	LEU	3.8
2	E	198	ILE	3.8
2	L	184	GLY	3.7
2	Q	125	PHE	3.7
1	F	473	GLY	3.7
1	D	581	ASN	3.7
2	Q	176	PHE	3.7
2	Q	164	TYR	3.7
2	L	174	ILE	3.6
1	F	550	ASN	3.6
2	Q	174	ILE	3.5
1	D	578	ALA	3.5
1	F	543	MET	3.5
2	Q	172	PHE	3.4
2	E	197	VAL	3.4
2	Q	189	TRP	3.4
2	Q	169	TYR	3.4
2	Q	188	THR	3.4
1	M	562	ILE	3.4
2	B	193	PHE	3.4
1	K	578	ALA	3.4
2	Q	165	VAL	3.3
2	Q	185	ASN	3.3
1	M	579	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	185	ASN	3.3
2	L	171	THR	3.3
2	B	157	VAL	3.3
2	Q	121	VAL	3.3
2	Q	180	CYS	3.2
1	K	585	TYR	3.2
2	Q	135	TYR	3.2
2	B	187	GLY	3.2
2	L	147	ALA	3.2
1	H	585	TYR	3.1
2	B	125	PHE	3.1
1	M	612	ASN	3.1
1	F	549	GLY	3.1
1	A	564	LEU	3.1
2	L	58	LEU	3.1
2	Q	147	ALA	3.1
2	B	191	VAL	3.1
2	L	173	TYR	3.0
2	B	134	THR	3.0
2	Q	145	THR	3.0
1	K	552	ILE	3.0
2	B	188	THR	3.0
2	L	169	TYR	3.0
2	J	193	PHE	3.0
1	H	627	LEU	3.0
2	L	121	VAL	3.0
1	F	517	LEU	3.0
1	M	580	ASP	3.0
2	B	189	TRP	3.0
2	Q	154	ALA	2.9
2	E	195	ASN	2.9
2	L	195	ASN	2.9
2	E	193	PHE	2.9
1	K	564	LEU	2.9
2	B	192	HIS	2.9
2	Q	143	TYR	2.9
2	J	157	VAL	2.9
2	Q	120	THR	2.9
2	Q	153	THR	2.9
2	Q	171	THR	2.9
2	B	124	TYR	2.9
2	J	169	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	Q	196	ASN	2.8
2	L	189	TRP	2.8
1	A	425	SER	2.8
2	J	35	GLN	2.8
1	F	548	ASP	2.8
2	Q	184	GLY	2.8
2	E	196	ASN	2.7
2	L	35	GLN	2.7
1	D	558	HIS	2.7
1	F	628	ASP	2.7
2	J	129	LYS	2.7
2	Q	142	TYR	2.7
2	J	123	VAL	2.7
2	L	156	CYS	2.7
2	Q	138	TRP	2.7
2	L	90	ALA	2.7
2	J	30	ILE	2.7
1	F	516	TRP	2.7
2	L	81	MET	2.7
2	L	188	THR	2.6
2	Q	136	VAL	2.6
2	Q	126	ASP	2.6
2	Q	113	CYS	2.6
1	H	552	ILE	2.6
1	F	435	PHE	2.5
2	B	122	GLN	2.5
2	J	143	TYR	2.5
1	D	556	ARG	2.5
1	A	522	ASP	2.5
1	H	551	PRO	2.5
1	M	563	GLN	2.5
2	L	172	PHE	2.5
2	Q	42	TRP	2.5
2	L	194	GLY	2.5
1	K	579	LYS	2.5
2	L	126	ASP	2.5
1	F	541	THR	2.5
1	F	545	ASN	2.5
1	F	612	ASN	2.5
1	D	629	LEU	2.5
1	A	554	ILE	2.5
2	B	123	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	Q	91	TYR	2.4
2	Q	186	THR	2.4
2	Q	114	PHE	2.4
1	A	562	ILE	2.4
1	M	554	ILE	2.4
2	G	199	ASP	2.4
2	J	165	VAL	2.4
2	L	187	GLY	2.4
2	L	176	PHE	2.4
2	Q	122	GLN	2.4
1	H	553	SER	2.4
2	B	186	THR	2.4
2	J	91	TYR	2.4
2	L	164	TYR	2.4
1	A	443	GLY	2.4
2	Q	187	GLY	2.4
2	J	141	VAL	2.4
2	Q	112	HIS	2.4
2	J	183	TYR	2.3
2	B	132	CYS	2.3
2	Q	183	TYR	2.3
2	E	51	ARG	2.3
2	L	165	VAL	2.3
2	Q	191	VAL	2.3
2	G	4	PRO	2.3
2	J	145	THR	2.3
1	M	618	CYS	2.3
2	J	118	GLY	2.3
2	J	151	ASP	2.3
2	J	155	THR	2.3
2	L	132	CYS	2.3
1	H	628	ASP	2.3
2	J	90	ALA	2.3
2	Q	137	ALA	2.3
2	E	127	GLY	2.3
2	J	81	MET	2.3
2	Q	163	TYR	2.3
2	L	159	HIS	2.2
1	F	520	LEU	2.2
2	Q	149	THR	2.2
2	Q	156	CYS	2.2
2	G	178	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	624	TRP	2.2
2	J	150	TRP	2.2
2	L	48	PHE	2.2
1	H	522	ASP	2.2
2	Q	141	VAL	2.2
2	L	54	GLY	2.2
1	F	514	HIS	2.2
2	Q	162	LEU	2.2
2	Q	140	SER	2.2
1	D	530	ASP	2.2
2	J	7	THR	2.2
2	Q	17	ASP	2.2
2	B	190	GLU	2.1
2	Q	157	VAL	2.1
2	E	56	GLN	2.1
2	J	162	LEU	2.1
2	B	183	TYR	2.1
1	F	521	THR	2.1
2	G	88	GLN	2.1
1	H	434	ARG	2.1
1	F	508	PHE	2.1
1	F	509	VAL	2.1
1	F	438	SER	2.1
1	M	438	SER	2.1
2	L	180	CYS	2.1
2	G	118	GLY	2.1
2	J	144	MET	2.0
2	E	74	HIS	2.0
2	Q	7	THR	2.0
2	E	169	TYR	2.0
2	E	10	GLU	2.0
2	L	150	TRP	2.0
1	F	519	PRO	2.0
1	M	584	PRO	2.0
2	Q	111	THR	2.0
1	M	585	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.