Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 11:12 PM EST

PDB ID	:	1TUE
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:

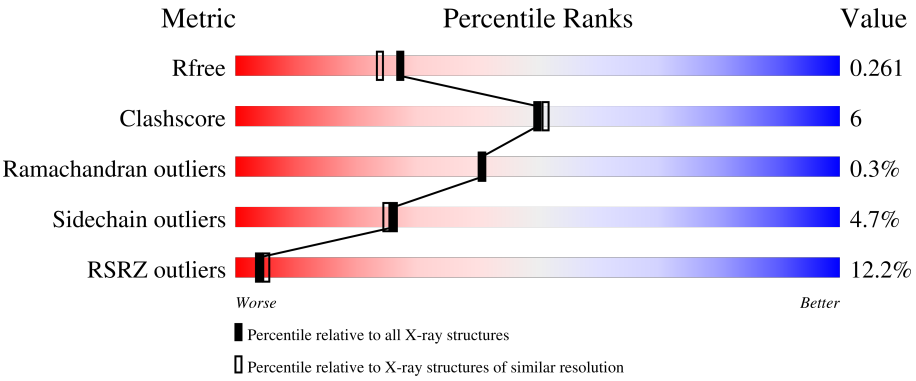
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	5% 77% 15% • 5%
1	D	212	5% 69% 23% •• 5%
1	F	212	20% 75% 13% • 11%
1	H	212	9% 72% 17% • 10%
1	K	212	8% 70% 19% • 9%

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Mol	Chain	Length	Quality of chain
1	M	212	8% 74% 17% 8%
2	B	218	9% 74% 13% 11%
2	E	218	5% 77% 13% 10%
2	G	218	6% 78% 10% 10%
2	J	218	12% 78% 10% 11%
2	L	218	22% 75% 13% 11%
2	Q	218	23% 79% 9% 11%

2 Entry composition (i)

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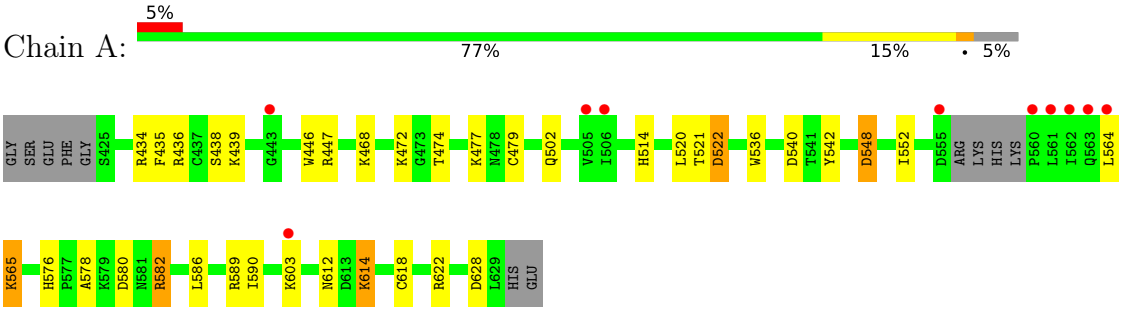
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	87	Total O 87 87	0	0
3	J	54	Total O 54 54	0	0
3	K	112	Total O 112 112	0	0
3	L	32	Total O 32 32	0	0
3	M	55	Total O 55 55	0	0
3	Q	29	Total O 29 29	0	0

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.

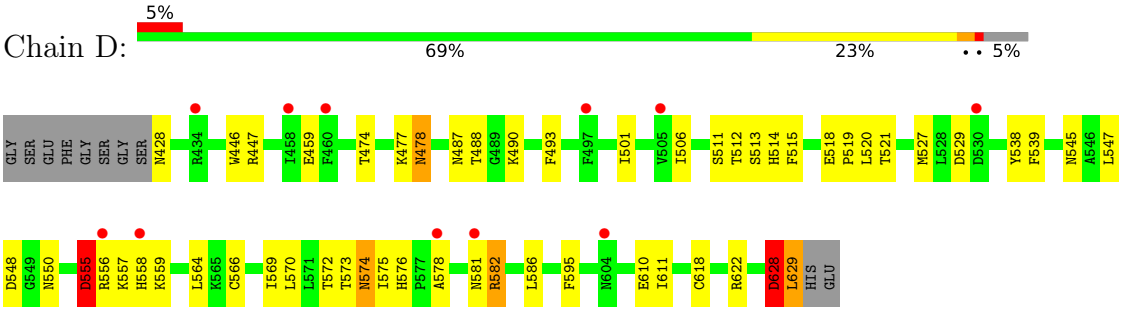
• Molecule 1: Replication protein E1

Chain A:



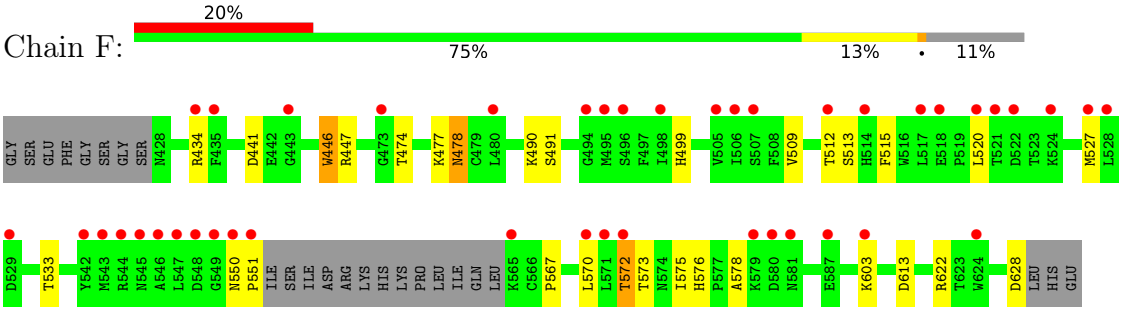
• Molecule 1: Replication protein E1

Chain D:



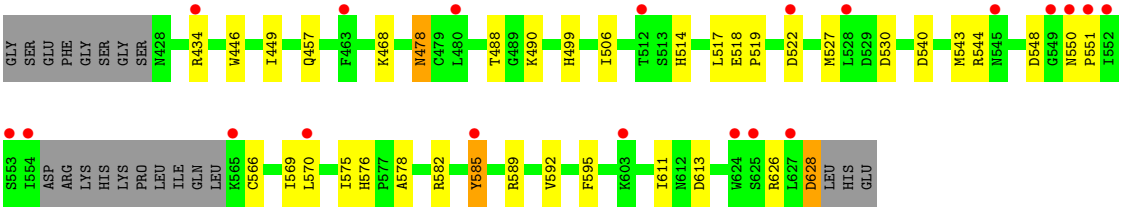
• Molecule 1: Replication protein E1

Chain F:



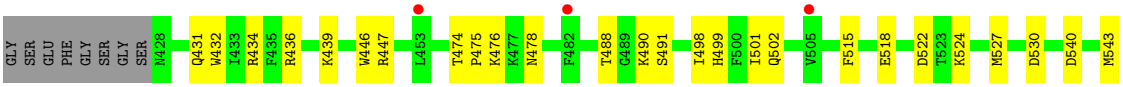
• Molecule 1: Replication protein E1

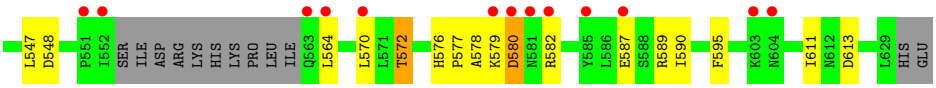
Chain H:



• Molecule 1: Replication protein E1

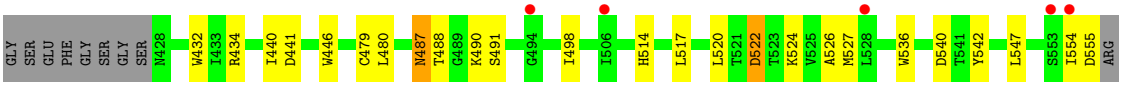
Chain K:

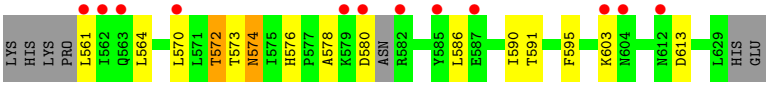




• Molecule 1: Replication protein E1

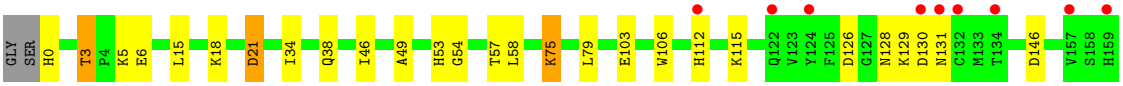
Chain M:

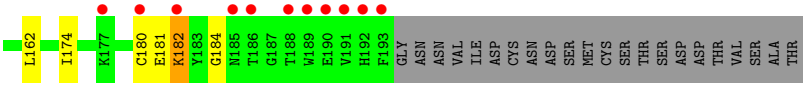




• Molecule 2: Regulatory protein E2

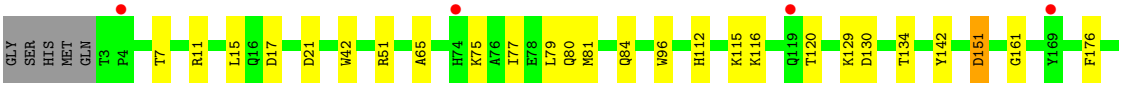
Chain B:

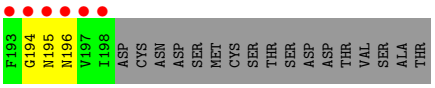




• Molecule 2: Regulatory protein E2

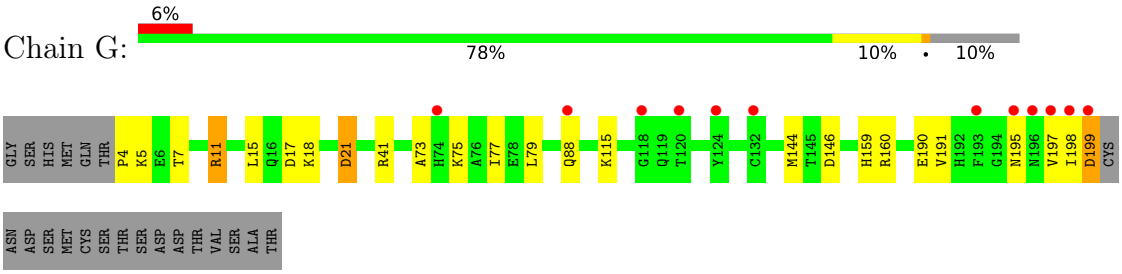
Chain E:





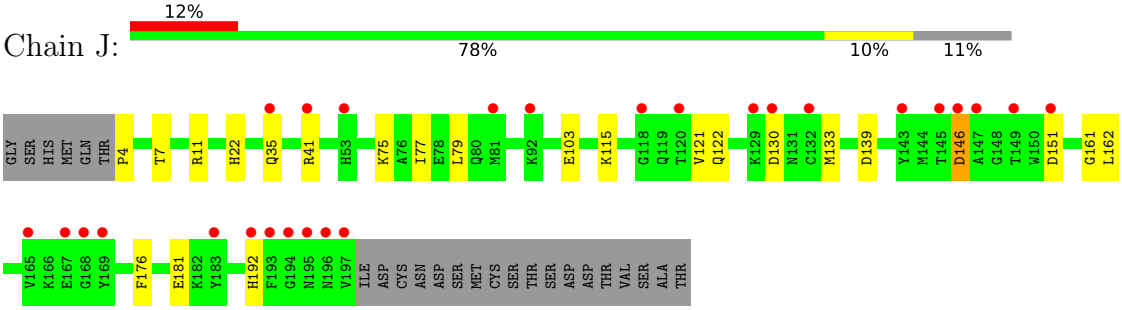
• Molecule 2: Regulatory protein E2

Chain G:



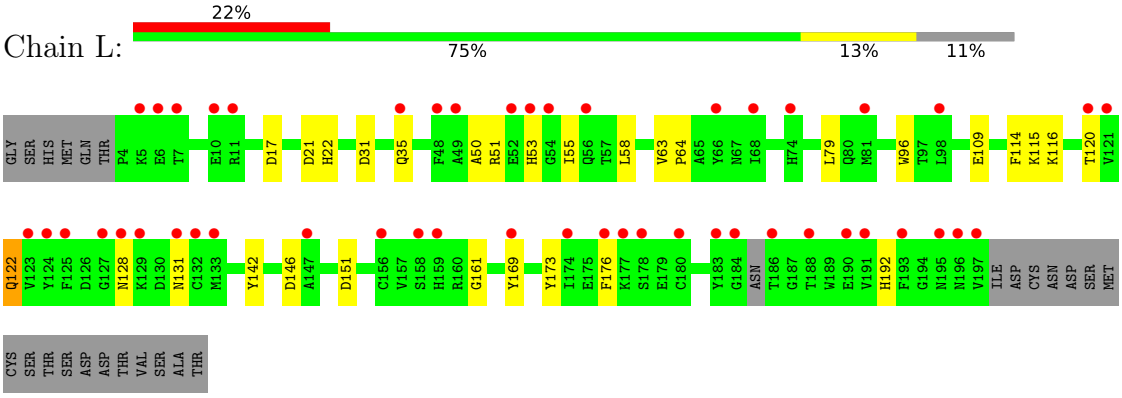
• Molecule 2: Regulatory protein E2

Chain J:



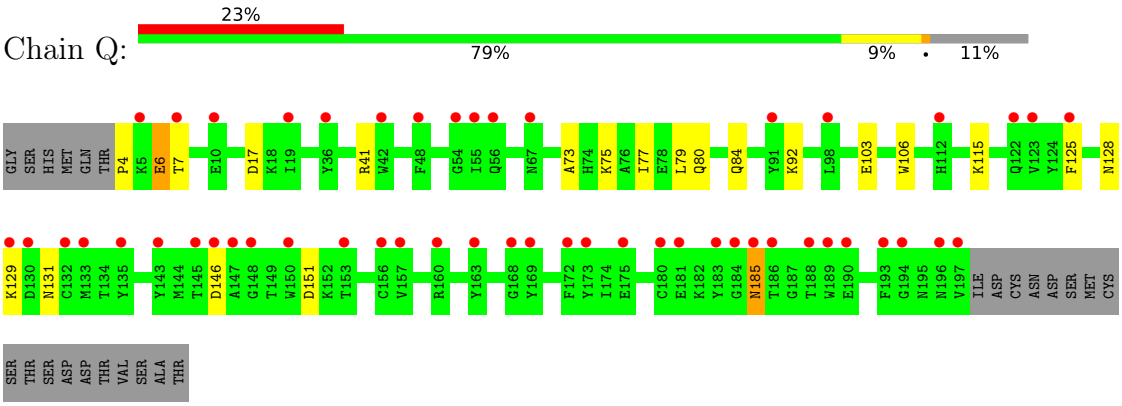
• Molecule 2: Regulatory protein E2

Chain L:



• Molecule 2: Regulatory protein E2

Chain Q:



4 Data and refinement statistics (i)

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 29.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.10) 99.0 (29.79-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.219 , 0.263 0.218 , 0.261	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)	0.33 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.47	0/1697	0.70	3/2304 (0.1%)
1	D	0.45	0/1722	0.70	4/2338 (0.2%)
1	F	0.40	0/1602	0.67	1/2175 (0.0%)
1	H	0.44	0/1624	0.68	5/2205 (0.2%)
1	K	0.44	0/1635	0.68	4/2220 (0.2%)
1	M	0.40	0/1664	0.67	5/2258 (0.2%)
2	B	0.41	0/1643	0.69	3/2229 (0.1%)
2	E	0.41	0/1650	0.70	3/2240 (0.1%)
2	G	0.39	0/1651	0.69	3/2240 (0.1%)
2	J	0.36	0/1635	0.66	3/2218 (0.1%)
2	L	0.35	0/1626	0.66	4/2204 (0.2%)
2	Q	0.34	0/1635	0.66	2/2218 (0.1%)
All	All	0.41	0/19784	0.68	40/26849 (0.1%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	130	ASP	CB-CG-OD2	6.74	124.37	118.30
2	B	146	ASP	CB-CG-OD2	6.29	123.96	118.30
1	H	540	ASP	CB-CG-OD2	6.27	123.94	118.30
1	H	522	ASP	CB-CG-OD2	6.12	123.81	118.30
2	J	130	ASP	CB-CG-OD2	6.04	123.74	118.30
1	M	555	ASP	CB-CG-OD2	5.91	123.62	118.30
2	G	146	ASP	CB-CG-OD2	5.89	123.60	118.30
1	D	628	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	540	ASP	CB-CG-OD2	5.67	123.41	118.30
2	E	130	ASP	CB-CG-OD2	5.63	123.37	118.30
1	H	530	ASP	CB-CG-OD2	5.56	123.31	118.30
1	K	580	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	522	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	555	ASP	CB-CG-OD2	5.48	123.23	118.30
2	B	21	ASP	CB-CG-OD2	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	146	ASP	CB-CG-OD2	5.45	123.20	118.30
1	H	548	ASP	CB-CG-OD2	5.45	123.20	118.30
2	G	21	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	548	ASP	CB-CG-OD2	5.43	123.18	118.30
2	E	17	ASP	CB-CG-OD2	5.38	123.14	118.30
1	M	540	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	151	ASP	CB-CG-OD2	5.29	123.06	118.30
1	K	540	ASP	CB-CG-OD2	5.24	123.01	118.30
2	L	151	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	529	ASP	CB-CG-OD2	5.22	123.00	118.30
1	K	522	ASP	CB-CG-OD2	5.21	122.99	118.30
2	Q	146	ASP	CB-CG-OD2	5.20	122.98	118.30
1	M	441	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	628	ASP	CB-CG-OD2	5.11	122.90	118.30
1	M	522	ASP	CB-CG-OD2	5.09	122.88	118.30
2	L	146	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	548	ASP	CB-CG-OD2	5.08	122.87	118.30
1	H	628	ASP	CB-CG-OD2	5.08	122.87	118.30
2	Q	151	ASP	CB-CG-OD2	5.07	122.86	118.30
2	G	199	ASP	CB-CG-OD2	5.07	122.86	118.30
2	L	17	ASP	CB-CG-OD2	5.05	122.85	118.30
1	K	548	ASP	CB-CG-OD2	5.05	122.84	118.30
1	M	580	ASP	CB-CG-OD2	5.05	122.84	118.30
2	J	139	ASP	CB-CG-OD2	5.02	122.82	118.30
2	L	31	ASP	CB-CG-OD2	5.00	122.80	118.30

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	20	0
1	D	1668	0	1632	33	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	22	0
2	B	1599	0	1496	18	0
2	E	1607	0	1504	11	0
2	G	1608	0	1502	24	0
2	J	1592	0	1487	9	0
2	L	1584	0	1480	15	0
2	Q	1592	0	1487	9	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	219	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 (219) 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
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:D:574:ASN:C	1:D:574:ASN:HD22	2.03	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
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
1:D:556:ARG:HB2	1:D:559:LYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:499:HIS:HD2	1:K:613:ASP:OD1	1.87	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:H:517:LEU:C	1:H:519:PRO:HD2	2.28	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: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
1:D:490:LYS:HE3	1:D:573:THR:O	2.11	0.51
1:D:513:SER:C	1:D:515:PHE:H	2.14	0.51
1:M:491:SER:OG	1:M:572:THR:HG21	2.11	0.51
2:B:180:CYS:C	2:B:182:LYS:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:CYS:O	1:A:622:ARG:HG3	2.12	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:51:ARG:C	2:L:53:HIS:H	2.19	0.46
2:E:80:GLN:O	2:E:84:GLN:HG3	2.15	0.46
2:B:126:ASP:C	2:B:128:ASN:H	2.18	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: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:M:487:ASN:C	1:M:487:ASN:HD22	2.21	0.44
1:D:513:SER:OG	1:D:515:PHE:HB3	2.18	0.44
1:F:447:ARG:NH2	2:G:21:ASP:OD1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:Q:4:PRO:N	2:Q:7:THR:HG1	2.17	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	15	11
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%)	15	11
2	E	194/218 (89%)	190 (98%)	3 (2%)	1 (0%)	29	26
2	G	194/218 (89%)	187 (96%)	6 (3%)	1 (0%)	29	26
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%)	29	26
All	All	2299/2580 (89%)	2230 (97%)	62 (3%)	7 (0%)	41	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	184	GLY
2	E	194	GLY
2	G	197	VAL

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Mol	Chain	Res	Type
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%)	28	28
1	D	184/191 (96%)	172 (94%)	12 (6%)	17	14
1	F	170/191 (89%)	162 (95%)	8 (5%)	26	25
1	H	173/191 (91%)	166 (96%)	7 (4%)	31	32
1	K	174/191 (91%)	165 (95%)	9 (5%)	23	21
1	M	178/191 (93%)	168 (94%)	10 (6%)	21	18
2	B	171/192 (89%)	162 (95%)	9 (5%)	22	20
2	E	172/192 (90%)	165 (96%)	7 (4%)	30	31
2	G	172/192 (90%)	163 (95%)	9 (5%)	23	21
2	J	170/192 (88%)	164 (96%)	6 (4%)	36	38
2	L	169/192 (88%)	164 (97%)	5 (3%)	41	44
2	Q	170/192 (88%)	163 (96%)	7 (4%)	30	31
All	All	2085/2298 (91%)	1988 (95%)	97 (5%)	26	25

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	LYS
1	A	446	TRP
1	A	520	LEU
1	A	552	ILE
1	A	565	LYS
1	A	582	ARG

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Mol	Chain	Res	Type
1	A	603	LYS
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
2	B	182	LYS
1	D	446	TRP
1	D	478	ASN
1	D	487	ASN
1	D	501	ILE
1	D	512	THR
1	D	555	ASP
1	D	558	HIS
1	D	574	ASN
1	D	575	ILE
1	D	582	ARG
1	D	628	ASP
1	D	629	LEU
2	E	75	LYS
2	E	79	LEU
2	E	112	HIS
2	E	115	LYS
2	E	129	LYS
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	572	THR
1	F	603	LYS
2	G	5	LYS
2	G	11	ARG
2	G	15	LEU
2	G	17	ASP

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Mol	Chain	Res	Type
2	G	18	LYS
2	G	75	LYS
2	G	79	LEU
2	G	115	LYS
2	G	195	ASN
1	H	434	ARG
1	H	446	TRP
1	H	478	ASN
1	H	490	LYS
1	H	575	ILE
1	H	585	TYR
1	H	628	ASP
2	J	79	LEU
2	J	115	LYS
2	J	133	MET
2	J	146	ASP
2	J	151	ASP
2	J	181	GLU
1	K	446	TRP
1	K	474	THR
1	K	478	ASN
1	K	501	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	115	LYS
2	L	120	THR
2	L	122	GLN
2	L	169	TYR
1	M	434	ARG
1	M	446	TRP
1	M	480	LEU
1	M	487	ASN
1	M	522	ASP
1	M	561	LEU
1	M	572	THR
1	M	574	ASN
1	M	591	THR
1	M	603	LYS

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Mol	Chain	Res	Type
2	Q	6	GLU
2	Q	79	LEU
2	Q	92	LYS
2	Q	115	LYS
2	Q	128	ASN
2	Q	129	LYS
2	Q	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	514	HIS
1	A	576	HIS
2	B	0	HIS
2	B	53	HIS
2	B	185	ASN
1	D	457	GLN
1	D	478	ASN
1	D	487	ASN
1	D	545	ASN
1	D	574	ASN
1	D	576	HIS
2	E	84	GLN
2	E	107	ASN
1	F	478	ASN
1	F	499	HIS
1	F	576	HIS
2	G	35	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
1	K	478	ASN
1	K	499	HIS
1	K	510	ASN
1	K	576	HIS
2	L	22	HIS
2	L	35	GLN
2	L	119	GLN

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Mol	Chain	Res	Type
2	L	128	ASN
1	M	487	ASN
1	M	499	HIS
1	M	514	HIS
1	M	574	ASN
1	M	576	HIS
2	Q	35	GLN
2	Q	84	GLN
2	Q	128	ASN
2	Q	131	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.34	10 (4%) 28 34	16, 25, 48, 68	0
1	D	202/212 (95%)	0.51	11 (5%) 25 31	20, 29, 44, 58	0
1	F	188/212 (88%)	1.40	43 (22%) 0 0	26, 42, 73, 96	0
1	H	191/212 (90%)	0.80	20 (10%) 6 8	20, 33, 53, 73	0
1	K	192/212 (90%)	0.51	16 (8%) 11 14	20, 33, 55, 62	0
1	M	196/212 (92%)	0.60	17 (8%) 10 13	30, 40, 56, 70	0
2	B	194/218 (88%)	0.56	20 (10%) 6 8	18, 32, 76, 83	0
2	E	196/218 (89%)	0.37	10 (5%) 28 33	21, 30, 49, 69	0
2	G	196/218 (89%)	0.44	12 (6%) 21 26	25, 36, 49, 71	0
2	J	194/218 (88%)	0.99	27 (13%) 2 3	26, 47, 67, 81	0
2	L	193/218 (88%)	1.27	48 (24%) 0 0	26, 52, 98, 101	0
2	Q	194/218 (88%)	1.52	51 (26%) 0 0	30, 60, 96, 101	0
All	All	2337/2580 (90%)	0.77	285 (12%) 4 5	16, 36, 75, 101	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	551	PRO	10.8
2	J	147	ALA	8.5
1	F	546	ALA	8.2
1	F	550	ASN	8.1
1	H	554	ILE	7.8
1	F	548	ASP	7.5
2	Q	183	TYR	7.2
2	L	125	PHE	7.2
1	F	542	TYR	7.1
2	J	193	PHE	7.1
2	Q	169	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
1	F	549	GLY	6.9
1	M	561	LEU	6.8
2	L	183	TYR	6.7
2	B	185	ASN	6.4
2	Q	125	PHE	6.4
2	L	169	TYR	6.3
2	Q	185	ASN	5.9
1	F	545	ASN	5.9
2	L	123	VAL	5.9
2	E	195	ASN	5.8
2	J	169	TYR	5.8
2	J	195	ASN	5.6
2	Q	156	CYS	5.6
1	F	543	MET	5.6
2	Q	196	ASN	5.5
2	Q	184	GLY	5.4
2	L	132	CYS	5.4
2	L	197	VAL	5.3
1	H	552	ILE	5.3
2	G	198	ILE	5.2
2	B	190	GLU	5.2
2	G	197	VAL	5.1
2	Q	193	PHE	4.9
1	M	562	ILE	4.8
2	Q	130	ASP	4.8
2	Q	180	CYS	4.8
2	Q	132	CYS	4.8
1	F	521	THR	4.7
1	M	579	LYS	4.7
2	B	159	HIS	4.6
1	F	512	THR	4.6
2	L	124	TYR	4.6
2	Q	194	GLY	4.5
2	L	193	PHE	4.5
2	E	194	GLY	4.5
1	M	604	ASN	4.4
1	H	551	PRO	4.3
2	J	194	GLY	4.3
2	J	129	LYS	4.3
2	L	178	SER	4.2
1	K	580	ASP	4.2
2	Q	172	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	561	LEU	4.1
2	L	190	GLU	4.1
1	A	555	ASP	4.1
2	J	130	ASP	4.1
2	Q	56	GLN	4.1
2	G	199	ASP	4.1
1	K	552	ILE	4.0
2	E	193	PHE	4.0
2	L	5	LYS	4.0
2	L	131	ASN	3.9
2	L	48	PHE	3.9
2	B	157	VAL	3.9
2	Q	123	VAL	3.9
1	K	603	LYS	3.8
2	Q	122	GLN	3.8
2	G	195	ASN	3.8
2	E	198	ILE	3.7
2	E	196	ASN	3.7
2	L	54	GLY	3.7
2	L	184	GLY	3.7
1	A	562	ILE	3.7
2	Q	163	TYR	3.7
1	A	603	LYS	3.7
2	J	167	GLU	3.6
1	K	585	TYR	3.6
2	J	118	GLY	3.6
1	F	581	ASN	3.6
2	Q	168	GLY	3.6
1	F	506	ILE	3.6
1	H	553	SER	3.6
2	L	127	GLY	3.6
2	L	56	GLN	3.5
1	D	581	ASN	3.5
2	Q	7	THR	3.5
2	Q	175	GLU	3.5
2	B	192	HIS	3.5
2	G	196	ASN	3.5
1	K	563	GLN	3.5
2	L	129	LYS	3.5
2	B	191	VAL	3.4
2	L	121	VAL	3.4
1	F	624	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	435	PHE	3.4
1	H	627	LEU	3.4
1	A	560	PRO	3.4
1	H	624	TRP	3.3
1	K	564	LEU	3.3
2	J	192	HIS	3.3
2	B	124	TYR	3.3
2	L	128	ASN	3.3
2	B	188	THR	3.3
2	Q	55	ILE	3.3
2	L	147	ALA	3.3
2	Q	173	TYR	3.3
2	Q	153	THR	3.2
1	F	443	GLY	3.2
2	Q	181	GLU	3.2
2	J	196	ASN	3.2
2	J	168	GLY	3.2
2	E	169	TYR	3.2
2	Q	188	THR	3.2
1	F	579	LYS	3.2
2	L	6	GLU	3.2
2	Q	42	TRP	3.2
1	F	505	VAL	3.2
2	J	197	VAL	3.2
2	L	188	THR	3.2
1	M	563	GLN	3.1
1	F	544	ARG	3.1
1	M	580	ASP	3.1
2	Q	112	HIS	3.1
2	Q	189	TRP	3.1
2	Q	5	LYS	3.1
1	F	527	MET	3.1
1	K	581	ASN	3.0
2	L	177	LYS	3.0
1	F	473	GLY	3.0
2	Q	150	TRP	3.0
2	Q	197	VAL	3.0
2	L	174	ILE	2.9
2	J	145	THR	2.9
1	F	518	GLU	2.9
2	J	149	THR	2.9
1	H	545	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	G	132	CYS	2.9
1	D	604	ASN	2.9
2	J	132	CYS	2.9
1	K	579	LYS	2.8
1	M	554	ILE	2.8
1	F	580	ASP	2.8
1	M	603	LYS	2.8
1	F	495	MET	2.8
1	F	520	LEU	2.8
1	H	565	LYS	2.8
2	Q	146	ASP	2.8
1	F	498	ILE	2.8
2	B	132	CYS	2.8
2	L	159	HIS	2.8
1	M	506	ILE	2.8
2	Q	133	MET	2.8
2	G	124	TYR	2.8
1	D	578	ALA	2.7
1	H	585	TYR	2.7
2	L	195	ASN	2.7
1	H	603	LYS	2.7
1	M	494	GLY	2.7
2	Q	145	THR	2.7
2	Q	186	THR	2.7
2	B	193	PHE	2.7
2	L	52	GLU	2.7
1	F	496	SER	2.7
1	H	434	ARG	2.7
1	H	522	ASP	2.7
2	B	189	TRP	2.7
1	F	528	LEU	2.7
1	F	565	LYS	2.7
2	Q	67	ASN	2.7
1	F	514	HIS	2.6
2	L	53	HIS	2.6
1	K	551	PRO	2.6
2	Q	160	ARG	2.6
2	Q	135	TYR	2.6
2	Q	157	VAL	2.6
2	Q	148	GLY	2.6
1	A	564	LEU	2.6
2	B	131	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	Q	129	LYS	2.5
1	F	434	ARG	2.5
1	D	558	HIS	2.5
2	J	165	VAL	2.5
1	K	604	ASN	2.5
2	G	88	GLN	2.5
1	K	453	LEU	2.5
1	A	505	VAL	2.5
1	F	603	LYS	2.5
2	Q	19	ILE	2.5
2	G	118	GLY	2.5
2	Q	48	PHE	2.5
2	J	35	GLN	2.5
2	L	156	CYS	2.5
1	F	570	LEU	2.4
2	E	74	HIS	2.4
2	Q	147	ALA	2.4
1	F	517	LEU	2.4
2	J	120	THR	2.4
1	H	528	LEU	2.4
1	M	528	LEU	2.4
1	D	458	ILE	2.4
2	L	186	THR	2.4
2	Q	91	TYR	2.4
2	B	180	CYS	2.4
2	L	158	SER	2.4
1	F	524	LYS	2.3
2	J	41	ARG	2.3
1	F	572	THR	2.3
2	J	183	TYR	2.3
2	E	4	PRO	2.3
2	Q	54	GLY	2.3
2	J	81	MET	2.3
1	F	480	LEU	2.3
2	L	176	PHE	2.3
2	J	146	ASP	2.3
1	F	547	LEU	2.3
2	L	98	LEU	2.3
1	K	482	PHE	2.3
1	K	587	GLU	2.3
2	Q	10	GLU	2.3
2	G	120	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	182	LYS	2.3
1	F	529	ASP	2.3
1	D	556	ARG	2.3
1	M	587	GLU	2.3
2	G	74	HIS	2.2
2	B	122	GLN	2.2
2	J	92	LYS	2.2
1	H	512	THR	2.2
1	H	463	PHE	2.2
1	M	582	ARG	2.2
2	L	196	ASN	2.2
2	J	151	ASP	2.2
2	B	112	HIS	2.2
1	D	497	PHE	2.2
1	M	585	TYR	2.2
2	Q	143	TYR	2.2
2	L	7	THR	2.2
1	D	460	PHE	2.2
1	K	582	ARG	2.2
2	L	133	MET	2.2
2	Q	98	LEU	2.2
2	L	66	TYR	2.2
2	B	134	THR	2.2
2	L	120	THR	2.2
1	A	506	ILE	2.1
1	D	530	ASP	2.1
2	B	186	THR	2.1
2	Q	190	GLU	2.1
1	F	571	LEU	2.1
1	H	570	LEU	2.1
2	B	177	LYS	2.1
2	G	193	PHE	2.1
1	F	494	GLY	2.1
2	L	81	MET	2.1
2	L	180	CYS	2.1
1	A	563	GLN	2.1
1	F	522	ASP	2.1
2	E	197	VAL	2.1
2	L	49	ALA	2.1
2	J	143	TYR	2.1
2	Q	36	TYR	2.1
2	L	10	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	549	GLY	2.1
1	K	570	LEU	2.1
1	M	553	SER	2.1
1	K	505	VAL	2.1
1	M	612	ASN	2.1
2	B	130	ASP	2.1
2	E	119	GLN	2.1
2	L	74	HIS	2.1
1	F	507	SER	2.0
1	H	550	ASN	2.0
1	H	480	LEU	2.0
2	L	68	ILE	2.0
2	J	53	HIS	2.0
1	A	443	GLY	2.0
1	D	434	ARG	2.0
1	H	625	SER	2.0
1	M	570	LEU	2.0
1	F	587	GLU	2.0
2	L	191	VAL	2.0
2	L	35	GLN	2.0
1	D	505	VAL	2.0
2	L	11	ARG	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 monosaccharides 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.