



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:13 PM EDT

PDB ID : 6F2R / pdb_00006f2r
Title : A heterotetramer of human HspB2 and HspB3
Authors : Clark, A.R.; Cole, A.R.; Boelens, W.C.; Keep, N.H.; Slingsby, C.
Deposited on : 2017-11-27
Resolution : 3.90 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

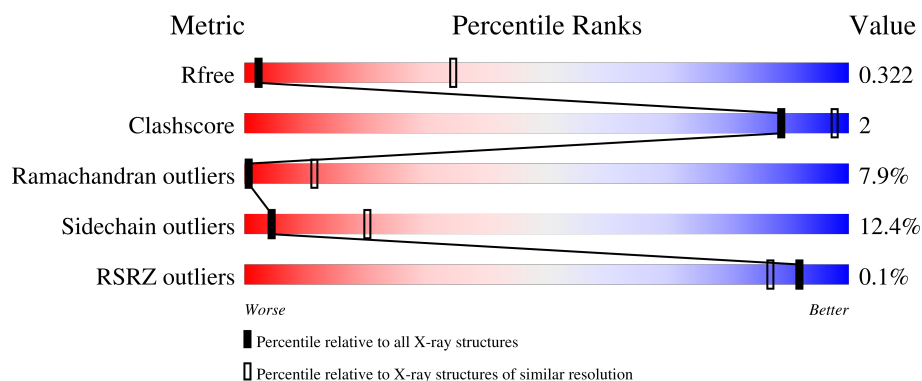
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



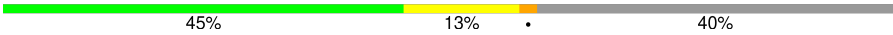
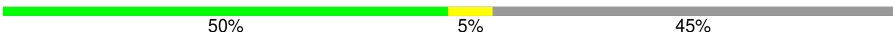
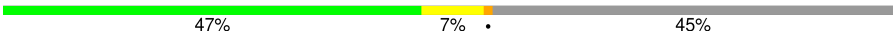
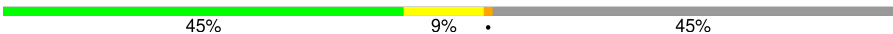
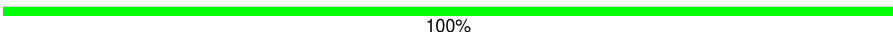
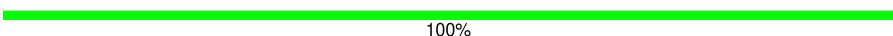
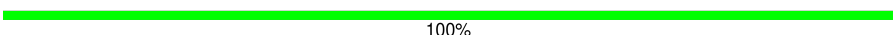
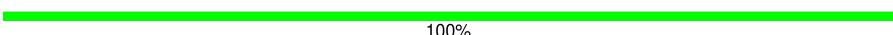
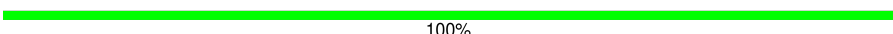
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	213	55% 6% 39%
1	E	213	54% 7% 39%
1	I	213	55% 5% 39%
2	C	203	49% 10% 40%
2	G	203	49% 9% 40%

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Mol	Chain	Length	Quality of chain
2	K	203	
3	D	182	
3	F	182	
3	J	182	
4	Q	161	
4	T	161	
4	V	161	
5	M	10	
6	N	7	
7	O	6	
8	1	5	
8	2	5	
8	3	5	
9	W	12	
9	X	12	
9	Y	12	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7592 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 HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			780	478	138	163	1			
1	E	130	Total	C	N	O	S	0	0	0
			777	475	138	163	1			
1	I	130	Total	C	N	O	S	0	0	0
			777	475	138	163	1			

- Molecule 2 is a protein called HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	121	Total	C	N	O	S	0	0	0
			796	498	141	156	1			
2	G	121	Total	C	N	O	S	0	0	0
			794	496	141	156	1			
2	K	121	Total	C	N	O	S	0	0	0
			796	498	141	156	1			

- Molecule 3 is a protein called Heat shock protein beta-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	80	Total	C	N	O	0	0	0
			406	246	80	80			
3	F	79	Total	C	N	O	0	0	0
			392	234	79	79			
3	J	79	Total	C	N	O	0	0	0
			392	234	79	79			

- Molecule 4 is a protein called Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	T	88	Total	C	N	O	0	0	0
			437	261	88	88			
4	V	88	Total	C	N	O	0	0	0
			437	261	88	88			
4	Q	89	Total	C	N	O	0	0	0
			443	265	89	89			

- Molecule 5 is a protein called Unknown peptide from HspB2 or HspB3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	10	Total	C	N	O	0	0	0
			46	26	10	10			

- Molecule 6 is a protein called Unknown peptide from HspB2 or HspB3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	7	Total	C	N	O	0	0	0
			35	21	7	7			

- Molecule 7 is a protein called Unknown peptide from HspB2 or HspB3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	O	6	Total	C	N	O	0	0	0
			30	18	6	6			

- Molecule 8 is a protein called Unknown peptide from HspB2 or HspB3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	1	5	Total	C	N	O	0	0	0
			25	15	5	5			
8	2	5	Total	C	N	O	0	0	0
			24	15	4	5			
8	3	5	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 9 is a protein called Unknown peptide from HspB2 or HspB3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	W	12	Total	C	N	O	0	0	0
			60	36	12	12			
9	X	12	Total	C	N	O	0	0	0
			60	36	12	12			

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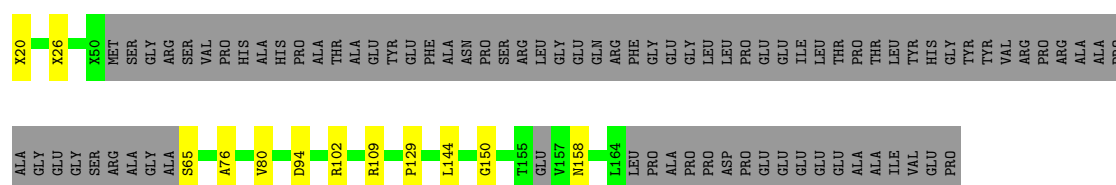
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Y	12	Total	C	N	O	0	0	0
			60	36	12	12			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

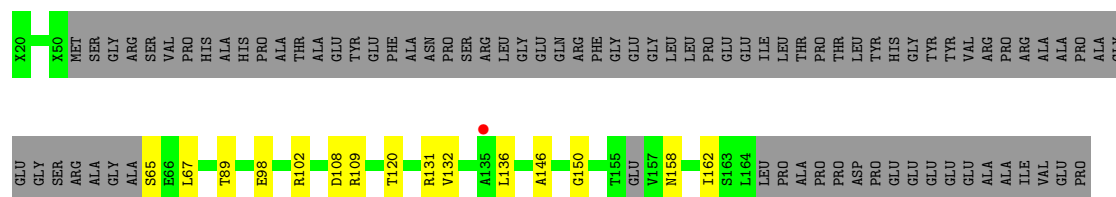
- Molecule 1: HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2

Chain A: 



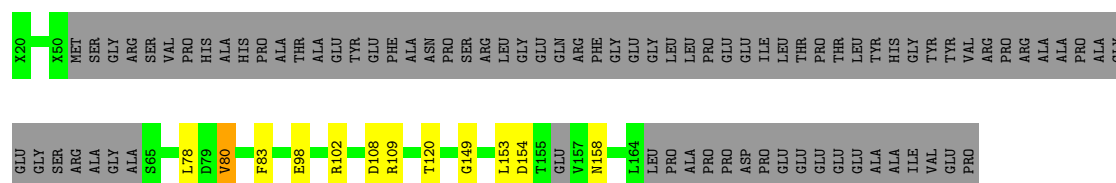
- Molecule 1: HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2

Chain E: 



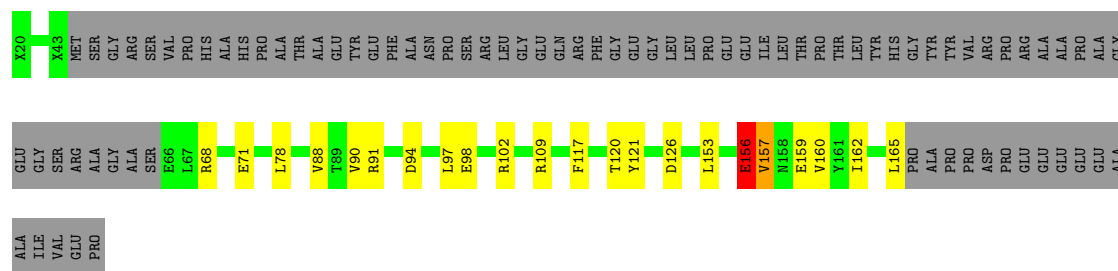
- Molecule 1: HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2

Chain I: 



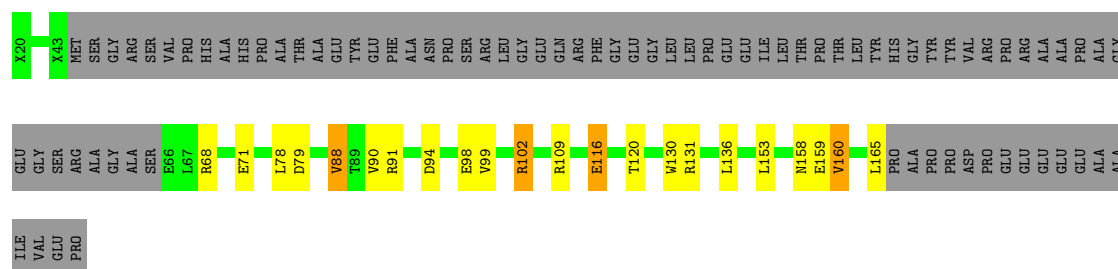
- Molecule 2: HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2

Chain C: 



- Molecule 2: HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2

Chain G: 49% 9% 40%



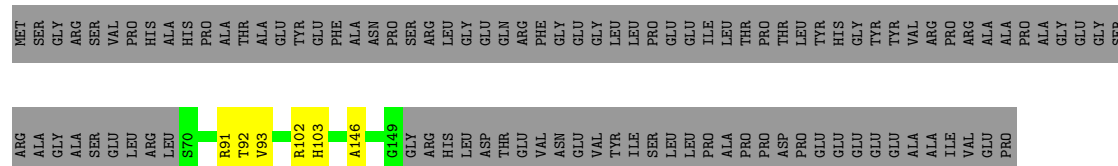
- Molecule 2: HspB2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2,Heat shock protein beta-2

Chain K: 45% 13% 40%



- Molecule 3: Heat shock protein beta-2

Chain D: 41% 56%



- Molecule 3: Heat shock protein beta-2

Chain F: 41% 57%

MET SER GLY ARG VAL PRO HIS ALA HIS PRO THR GLU TYR PHE ALA ASN PRO SER ARG LEU GLU GLN PHE GLY GLY LEU PRO PRO GLU ILE THR ASP THR LEU HIS TYR VAL ARG PRO ARG ALA GLY SER

ARG ALA GLY ALA SER GLU LEU ARG LEU S70 P129 V132 R133 P147 R148 GLY GLY ARG HIS LEU ASP THR GLU VAL ASN ARG PHE GLY VAL TYR ILE SER LEU LEU PRO GLU ALA PRO PRO THR ASP THR GLU LEU TYR HIS GLY TYR VAL ARG PRO ARG ALA ALA PRO PRO GLY GLY SER

- Molecule 3: Heat shock protein beta-2

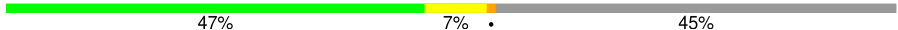
Chain J:  37% 5% 57%

MET SER GLY ARG VAL PRO HIS ALA HIS PRO THR GLU TYR PHE ALA ASN PRO SER ARG LEU GLU GLN PHE GLY GLY LEU PRO PRO GLU ILE THR ASP THR LEU TYR HIS GLY TYR VAL ARG PRO ARG ALA ALA PRO PRO GLY GLY SER

ARG ALA GLY ALA SER GLU LEU ARG LEU S70 K73 F74 Q75 V80 D94 R106 H110 D128 P129 A135 E145 A146 P147 R148 GLY GLY ARG HIS LEU ASP THR THR VAL TYR SER LEU PRO ALA PRO ASP ASP ALA GLU GLU GLU GLU

ALA ILE VAL GLU PRO

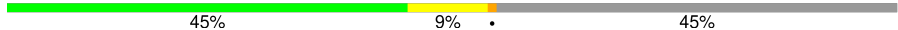
- Molecule 4: Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-2

Chain T:  47% 7% 45%

H1 A2 H8 L9 I10 GLU ILE PRO VAL ARG TYR GLN GLU PHE GLU ALA ARG GLY LEU ASP HIS ALA LEU TYR ALA PRO GLY PRO THR ILE VAL ASP LEU ARG LYS THR ARG ALA ALA GLN SER PRO VAL ASP SER ALA ALA GLU THR PRO

ARG GLU G67 K68 I85 E91 G92 Q99 H100 D105 V124 E125 I126 V143 R144 ASP VAL THR PRO GLU GLU GLU GLU ALA ILE VAL GLU PRO

- Molecule 4: Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-2

Chain V:  45% 9% 45%

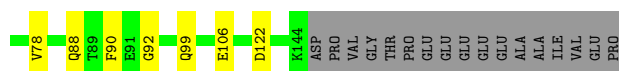
H1 A2 R7 H8 L9 I10 GLU ILE PRO VAL ARG TYR GLN GLU PHE GLU ALA ARG GLY LEU GLU ASP CYS ARG LEU HIS ALA LEU TYR ALA PRO GLY PRO THR ILE VAL ASP LEU ARG LYS THR ARG ALA ALA GLN SER PRO VAL ASP SER ALA ALA GLU THR PRO

PRO ARG GLU G67 K68 S69 I87 E91 A98 Q99 H100 F114 E125 D128 A131 G137 V143 R144 ASP PRO VAL GLY THR PRO GLU GLU GLU GLU ALA ILE VAL GLU PRO

- Molecule 4: Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-3,Heat shock protein beta-2

Chain Q:  50% 5% 45%

H1 I9 I10 GLU ILE VAL PRO ARG TYR GLN GLU PHE GLU ALA ARG GLY LEU GLU ASP CYS ARG LEU LEU HIS ALA TYR ALA PRO GLY PRO THR ILE VAL ASP LEU ARG LYS THR ARG ALA ALA GLN SER PRO VAL ASP SER ALA ALA GLU THR PRO ARG



- Molecule 5: Unknown peptide from HspB2 or HspB3

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Unknown peptide from HspB2 or HspB3

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Unknown peptide from HspB2 or HspB3

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Unknown peptide from HspB2 or HspB3

Chain 1:  80% 20%



- Molecule 8: Unknown peptide from HspB2 or HspB3

Chain 2:  60% 40%



- Molecule 8: Unknown peptide from HspB2 or HspB3

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown peptide from HspB2 or HspB3

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown peptide from HspB2 or HspB3

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Unknown peptide from HspB2 or HspB3

Chain Y:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	177.14Å 177.14Å 126.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	78.00 – 3.90 78.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (78.00-3.90) 99.8 (78.00-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.89Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.297 , 0.313 0.299 , 0.322	Depositor DCC
R_{free} test set	2088 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	158.1	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 371.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l 0.358 for h,-h-k,-l 0.087 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7592	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

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	0.77	0/632	1.18	0/876
1	E	0.77	0/632	1.15	0/876
1	I	0.83	0/632	1.18	0/876
2	C	0.80	0/708	1.28	2/975 (0.2%)
2	G	0.84	0/708	1.21	0/975
2	K	0.84	0/708	1.28	2/975 (0.2%)
3	D	0.76	0/408	1.18	0/568
3	F	0.92	0/393	1.52	2/546 (0.4%)
3	J	0.93	0/393	1.48	7/546 (1.3%)
4	Q	0.89	0/443	1.39	0/615
4	T	0.91	0/437	1.42	1/606 (0.2%)
4	V	0.92	0/437	1.34	0/606
All	All	0.84	0/6531	1.29	14/9040 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2
4	T	0	3
4	V	0	5
All	All	0	10

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	129	PRO	N-CA-CB	13.10	111.43	102.79
2	C	156	GLU	CA-C-N	9.14	138.16	121.70
2	C	156	GLU	C-N-CA	9.14	138.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	156	GLU	CA-C-N	8.66	137.29	121.70
2	K	156	GLU	C-N-CA	8.66	137.29	121.70
3	J	147	PRO	N-CA-CB	7.56	111.19	103.25
3	J	129	PRO	N-CA-CB	7.23	111.29	103.33
3	F	147	PRO	N-CA-CB	6.50	110.08	103.25
4	T	126	ILE	N-CA-CB	-5.60	103.47	110.47
3	J	146	ALA	CA-C-N	5.45	126.65	119.84
3	J	146	ALA	C-N-CA	5.45	126.65	119.84
3	J	128	ASP	CA-C-N	5.29	124.92	119.05
3	J	128	ASP	C-N-CA	5.29	124.92	119.05
3	J	106	ARG	N-CA-C	5.16	113.71	108.75

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	103	HIS	Mainchain
3	D	146	ALA	Mainchain
4	T	100	HIS	Peptide
4	T	143	VAL	Peptide,Mainchain
4	V	100	HIS	Peptide,Mainchain
4	V	125	GLU	Peptide,Mainchain
4	V	143	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	780	0	533	3	0
1	E	777	0	533	2	0
1	I	777	0	533	3	0
2	C	796	0	623	3	0
2	G	794	0	621	4	0
2	K	796	0	622	4	0
3	D	406	0	195	0	0
3	F	392	0	181	0	0
3	J	392	0	181	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	443	0	204	1	0
4	T	437	0	201	0	0
4	V	437	0	201	2	0
5	M	46	0	10	0	0
6	N	35	0	9	0	0
7	O	30	0	8	0	0
8	1	25	0	7	1	0
8	2	24	0	7	1	0
8	3	25	0	7	0	0
9	W	60	0	15	0	0
9	X	60	0	17	0	0
9	Y	60	0	17	0	0
All	All	7592	0	4725	23	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 2.

All (23) 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)
8:2:3:UNK:C	8:2:4:UNK:CA	2.56	0.83
3:J:75:GLN:HA	3:J:145:GLU:HA	1.81	0.62
2:G:131:ARG:HH22	1:I:154:ASP:H	1.51	0.57
4:Q:88:GLN:HA	8:1:1:UNK:HA	1.85	0.57
2:K:66:GLU:N	2:K:121:TYR:HH	2.02	0.56
1:A:76:ALA:HB3	1:A:144:LEU:HB2	1.90	0.54
2:C:97:LEU:HB3	2:C:121:TYR:HB2	1.91	0.53
3:J:73:LYS:HA	3:J:147:PRO:HA	1.90	0.53
2:G:130:TRP:HZ2	2:K:150:GLY:H	1.61	0.49
1:A:20:UNK:HA	1:A:26:UNK:HA	1.94	0.49
4:V:7:ARG:H	3:J:135:ALA:HA	1.78	0.48
2:G:102:ARG:HA	2:G:116:GLU:HA	1.96	0.46
1:A:94:ASP:O	1:A:129:PRO:HB3	2.16	0.45
2:G:98:GLU:HG3	2:G:120:THR:HB	2.00	0.44
4:V:98:ALA:HB3	4:V:114:PHE:H	1.82	0.44
1:E:98:GLU:HA	1:E:120:THR:HA	1.99	0.43
1:E:132:VAL:HG13	1:E:146:ALA:HB2	2.00	0.43
1:I:80:VAL:HG12	1:I:83:PHE:HB2	2.00	0.42
2:K:98:GLU:HG3	2:K:120:THR:HB	2.02	0.42
1:I:98:GLU:HA	1:I:120:THR:HG22	2.01	0.41
2:K:156:GLU:HA	2:K:157:VAL:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:GLU:HA	2:C:120:THR:HA	2.02	0.41
2:C:156:GLU:HA	2:C:157:VAL:O	2.20	0.41

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	95/213 (45%)	76 (80%)	15 (16%)	4 (4%)	2	20
1	E	95/213 (45%)	75 (79%)	14 (15%)	6 (6%)	1	15
1	I	95/213 (45%)	76 (80%)	14 (15%)	5 (5%)	1	17
2	C	98/203 (48%)	76 (78%)	12 (12%)	10 (10%)	0	7
2	G	98/203 (48%)	76 (78%)	14 (14%)	8 (8%)	0	11
2	K	98/203 (48%)	70 (71%)	16 (16%)	12 (12%)	0	4
3	D	78/182 (43%)	67 (86%)	7 (9%)	4 (5%)	1	17
3	F	77/182 (42%)	60 (78%)	14 (18%)	3 (4%)	2	21
3	J	77/182 (42%)	59 (77%)	13 (17%)	5 (6%)	1	15
4	Q	85/161 (53%)	63 (74%)	15 (18%)	7 (8%)	0	11
4	T	84/161 (52%)	59 (70%)	15 (18%)	10 (12%)	0	4
4	V	84/161 (52%)	62 (74%)	12 (14%)	10 (12%)	0	4
All	All	1064/2277 (47%)	819 (77%)	161 (15%)	84 (8%)	1	11

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	157	VAL
4	T	124	VAL

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Mol	Chain	Res	Type
2	G	160	VAL
4	V	69	SER
2	K	157	VAL
4	Q	78	VAL
3	F	147	PRO
3	J	145	GLU
3	J	147	PRO
2	C	68	ARG
2	C	153	LEU
2	C	159	GLU
2	C	160	VAL
4	T	91	GLU
2	G	68	ARG
1	I	153	LEU
4	V	91	GLU
4	V	131	ALA
4	V	143	VAL
2	K	108	ASP
2	K	153	LEU
2	K	159	GLU
2	K	160	VAL
2	C	71	GLU
2	C	94	ASP
3	D	102	ARG
1	E	108	ASP
1	E	158	ASN
4	T	2	ALA
4	T	105	ASP
2	G	94	ASP
2	G	153	LEU
1	I	108	ASP
1	I	109	ARG
4	V	137	GLY
2	K	68	ARG
2	K	81	SER
2	K	94	ASP
4	Q	92	GLY
1	A	158	ASN
3	D	91	ARG
1	E	102	ARG
1	E	150	GLY
4	T	8	HIS

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Mol	Chain	Res	Type
4	T	68	LYS
2	G	71	GLU
2	G	102	ARG
2	G	109	ARG
4	V	8	HIS
2	K	71	GLU
4	Q	99	GLN
4	Q	122	ASP
3	F	132	VAL
3	F	133	ARG
3	J	94	ASP
1	A	102	ARG
1	A	109	ARG
2	C	102	ARG
2	C	156	GLU
3	D	93	VAL
1	E	109	ARG
1	E	131	ARG
4	T	99	GLN
4	T	143	VAL
1	I	102	ARG
4	V	2	ALA
4	V	99	GLN
2	K	102	ARG
4	Q	9	LEU
4	Q	106	GLU
3	J	110	HIS
2	C	109	ARG
3	D	92	THR
4	V	128	ASP
4	Q	90	PHE
4	T	85	ILE
2	K	104	PRO
2	K	150	GLY
2	G	88	VAL
1	I	149	GLY
1	A	150	GLY
4	V	87	ILE
3	J	80	VAL
4	T	92	GLY

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	52/151 (34%)	50 (96%)	2 (4%)	29	52
1	E	52/151 (34%)	47 (90%)	5 (10%)	8	29
1	I	52/151 (34%)	49 (94%)	3 (6%)	18	44
2	C	62/151 (41%)	54 (87%)	8 (13%)	4	20
2	G	62/151 (41%)	50 (81%)	12 (19%)	1	9
2	K	62/151 (41%)	48 (77%)	14 (23%)	1	5
3	D	3/151 (2%)	3 (100%)	0	100	100
3	F	2/151 (1%)	2 (100%)	0	100	100
3	J	2/151 (1%)	2 (100%)	0	100	100
4	Q	2/140 (1%)	2 (100%)	0	100	100
4	T	2/140 (1%)	2 (100%)	0	100	100
4	V	2/140 (1%)	2 (100%)	0	100	100
All	All	355/1779 (20%)	311 (88%)	44 (12%)	4	20

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	80	VAL
2	C	78	LEU
2	C	88	VAL
2	C	90	VAL
2	C	91	ARG
2	C	117	PHE
2	C	126	ASP
2	C	162	ILE
2	C	165	LEU
1	E	65	SER
1	E	67	LEU
1	E	89	THR
1	E	136	LEU

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Mol	Chain	Res	Type
1	E	162	ILE
2	G	78	LEU
2	G	79	ASP
2	G	88	VAL
2	G	90	VAL
2	G	91	ARG
2	G	99	VAL
2	G	116	GLU
2	G	136	LEU
2	G	158	ASN
2	G	159	GLU
2	G	160	VAL
2	G	165	LEU
1	I	78	LEU
1	I	80	VAL
1	I	158	ASN
2	K	78	LEU
2	K	88	VAL
2	K	89	THR
2	K	97	LEU
2	K	103	HIS
2	K	105	GLN
2	K	116	GLU
2	K	123	LEU
2	K	136	LEU
2	K	141	ILE
2	K	159	GLU
2	K	162	ILE
2	K	164	LEU
2	K	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
2	C	103	HIS
1	I	158	ASN
2	K	110	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	K	1
2	C	1
2	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	32:UNK	C	36:UNK	N	10.50
1	C	32:UNK	C	36:UNK	N	10.44
1	G	32:UNK	C	36:UNK	N	8.90

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	99/213 (46%)	-0.72	0	100	100	86, 126, 176, 199	0
1	E	99/213 (46%)	-0.71	1 (1%)	79	59	84, 140, 194, 213	0
1	I	99/213 (46%)	-0.80	0	100	100	116, 158, 196, 210	0
2	C	100/203 (49%)	-0.72	0	100	100	100, 174, 205, 220	0
2	G	100/203 (49%)	-0.74	0	100	100	86, 150, 194, 211	0
2	K	100/203 (49%)	-0.74	0	100	100	115, 155, 211, 249	0
3	D	80/182 (43%)	-0.72	0	100	100	100, 164, 213, 221	0
3	F	79/182 (43%)	-1.04	0	100	100	71, 106, 147, 158	0
3	J	79/182 (43%)	-0.84	0	100	100	86, 113, 155, 172	0
4	Q	89/161 (55%)	-1.03	0	100	100	65, 93, 160, 192	0
4	T	88/161 (54%)	-0.78	0	100	100	92, 148, 200, 229	0
4	V	88/161 (54%)	-0.83	0	100	100	106, 147, 205, 221	0
5	M	0/10	-	-	-	-	-	-
6	N	0/7	-	-	-	-	-	-
7	O	0/6	-	-	-	-	-	-
8	1	0/5	-	-	-	-	-	-
8	2	0/5	-	-	-	-	-	-
8	3	0/5	-	-	-	-	-	-
9	W	0/12	-	-	-	-	-	-
9	X	0/12	-	-	-	-	-	-
9	Y	0/12	-	-	-	-	-	-
All	All	1100/2351 (46%)	-0.80	1 (0%)	92	87	65, 143, 201, 249	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	135	ALA	2.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.