



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 03:08 AM EDT

PDB ID : 5MK1  
Title : Crystal structure of the His Domain Protein Tyrosine Phosphatase (HD-PTP/PTPN23) Bro1 domain (CHMP4A peptide complex structure)  
Authors : Levy, C.; Gahloth, D.  
Deposited on : 2016-12-02  
Resolution : 2.50 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](mailto: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>.

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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	:	2.37.1
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)	:	2.37.1

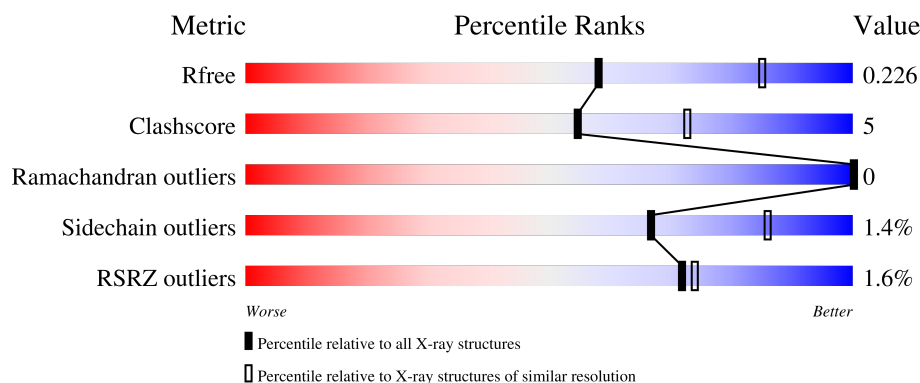
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	361	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	B	361	<div> <div>87%</div> <div>12%</div> <div>..</div> </div>
1	C	361	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	D	361	<div> <div>87%</div> <div>12%</div> <div>..</div> </div>
2	E	18	<div> <div>6%</div> <div>50%</div> <div>11%</div> <div>39%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	18	<div><div><div></div><div></div><div></div><div></div></div><div>6%39%22%39%</div></div>
2	H	18	<div><div><div></div><div></div><div></div><div></div></div><div>28%50%11%39%</div></div>
2	K	18	<div><div><div></div><div></div><div></div><div></div></div><div>6%39%17%6%39%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11890 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 Tyrosine-protein phosphatase non-receptor type 23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2835	1813	487	517	18			
1	B	358	Total	C	N	O	S	0	0	0
			2835	1813	487	517	18			
1	C	361	Total	C	N	O	S	0	0	0
			2857	1826	490	522	19			
1	D	359	Total	C	N	O	S	0	0	0
			2840	1816	488	518	18			

- Molecule 2 is a protein called Charged multivesicular body protein 4a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			89	58	14	17			
2	F	11	Total	C	N	O	0	0	0
			89	58	14	17			
2	H	11	Total	C	N	O	0	0	0
			89	58	14	17			
2	K	11	Total	C	N	O	0	0	0
			89	58	14	17			

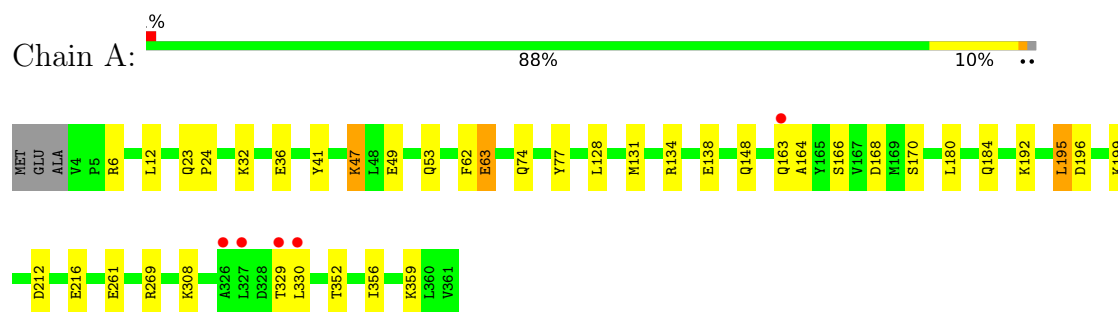
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total	O	0	0
			59	59		
3	B	24	Total	O	0	0
			24	24		
3	C	48	Total	O	0	0
			48	48		
3	D	36	Total	O	0	0
			36	36		

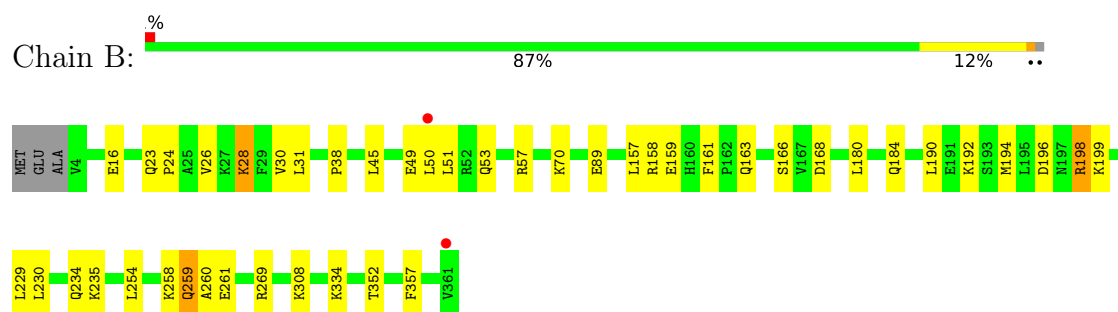
### 3 Residue-property plots

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.

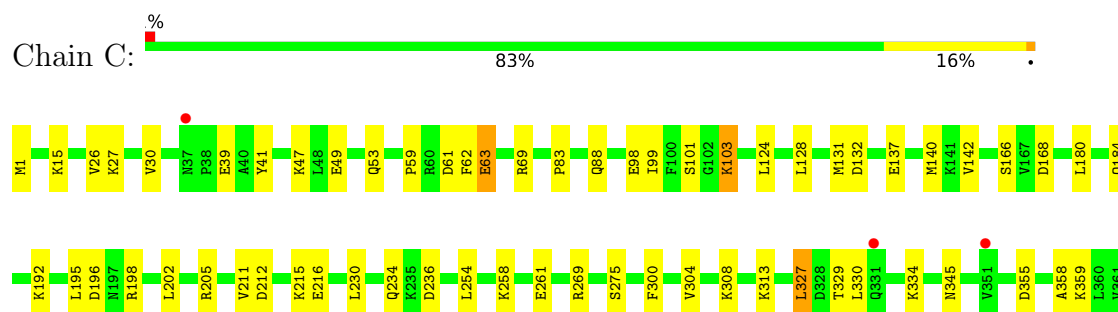
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 23



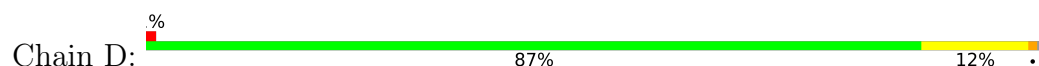
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 23

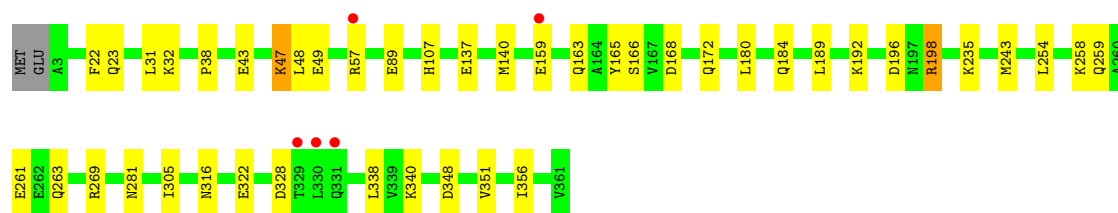


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 23

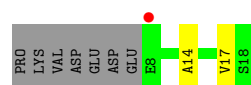


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 23

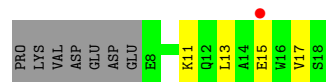




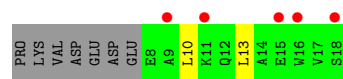
• Molecule 2: Charged multivesicular body protein 4a



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• Molecule 2: Charged multivesicular body protein 4a



• Molecule 2: Charged multivesicular body protein 4a



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.46Å 73.67Å 79.38Å 114.43° 90.28° 104.20°	Depositor
Resolution (Å)	28.41 – 2.50 28.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (28.41-2.50) 93.1 (28.96-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11_2563: ???)	Depositor
R, $R_{free}$	0.176 , 0.226 0.176 , 0.226	Depositor DCC
$R_{free}$ test set	1771 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.39	1/2897 (0.0%)	0.66	10/3914 (0.3%)
1	B	0.39	0/2897	0.63	4/3914 (0.1%)
1	C	0.35	0/2918	0.62	8/3940 (0.2%)
1	D	0.35	0/2902	0.69	8/3921 (0.2%)
2	E	0.28	0/90	0.49	0/121
2	F	0.29	0/90	0.63	0/121
2	H	0.34	0/90	0.65	0/121
2	K	0.48	0/90	0.57	0/121
All	All	0.37	1/11974 (0.0%)	0.65	30/16173 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	GLU	CD-OE1	-5.63	1.19	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	ARG	CB-CG-CD	-18.36	63.87	111.60
1	B	57	ARG	CB-CG-CD	-13.04	77.70	111.60
1	A	32	LYS	CD-CE-NZ	-10.78	86.90	111.70
1	C	63	GLU	N-CA-CB	10.39	129.31	110.60
1	B	50	LEU	CB-CG-CD2	-10.32	93.45	111.00
1	D	43	GLU	CA-CB-CG	10.13	135.69	113.40
1	C	63	GLU	CB-CA-C	-9.07	92.26	110.40
1	D	47	LYS	CD-CE-NZ	-8.56	92.02	111.70
1	D	57	ARG	CA-CB-CG	8.44	131.97	113.40
1	A	195	LEU	CB-CG-CD2	7.54	123.82	111.00
1	D	43	GLU	CB-CA-C	7.35	125.09	110.40
1	C	63	GLU	CB-CG-CD	-7.27	94.58	114.20
1	D	163	GLN	N-CA-CB	-6.96	98.08	110.60
1	A	32	LYS	CA-CB-CG	6.86	128.49	113.40
1	B	50	LEU	CA-CB-CG	6.80	130.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	ARG	CG-CD-NE	6.79	126.06	111.80
1	C	63	GLU	CA-CB-CG	6.65	128.04	113.40
1	C	103	LYS	CA-CB-CG	6.62	127.96	113.40
1	A	36	GLU	CA-CB-CG	6.62	127.95	113.40
1	D	172	GLN	CA-CB-CG	6.46	127.60	113.40
1	A	62	PHE	C-N-CA	-6.44	105.61	121.70
1	B	57	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	138	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	C	62	PHE	C-N-CA	-5.87	107.03	121.70
1	A	47	LYS	CD-CE-NZ	-5.58	98.85	111.70
1	A	195	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	C	327	LEU	CA-CB-CG	-5.39	102.89	115.30
1	A	63	GLU	N-CA-CB	5.26	120.08	110.60
1	C	103	LYS	CD-CE-NZ	5.13	123.50	111.70
1	A	32	LYS	CB-CG-CD	-5.09	98.36	111.60

There are no chirality outliers.

There are no planarity outliers.

## 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	2835	0	2850	28	0
1	B	2835	0	2850	31	0
1	C	2857	0	2872	36	1
1	D	2840	0	2855	24	1
2	E	89	0	88	3	0
2	F	89	0	88	3	0
2	H	89	0	88	2	0
2	K	89	0	88	3	0
3	A	59	0	0	0	0
3	B	24	0	0	1	0
3	C	48	0	0	0	0
3	D	36	0	0	0	0
All	All	11890	0	11779	121	1

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 5.

All (121) 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:A:329:THR:HG23	1:A:330:LEU:HD23	1.53	0.89
1:A:329:THR:HG23	1:A:330:LEU:CD2	2.02	0.89
1:B:234:GLN:OE1	1:B:235:LYS:HD2	1.81	0.79
1:D:198:ARG:NH2	2:K:12:GLN:OE1	2.17	0.77
1:A:77:TYR:CE1	1:A:352:THR:HG21	2.20	0.76
1:D:23:GLN:NE2	1:D:49:GLU:OE1	2.19	0.73
1:A:329:THR:C	1:A:330:LEU:HD22	2.10	0.72
1:A:63:GLU:OE2	1:C:142:VAL:HG21	1.90	0.71
1:D:47:LYS:HD3	1:D:356:ILE:HG12	1.74	0.70
2:F:11:LYS:O	2:F:15:GLU:HG2	1.92	0.70
1:A:74:GLN:HE22	1:A:356:ILE:H	1.43	0.67
1:B:261:GLU:HB2	1:B:269:ARG:HD2	1.80	0.63
1:A:163:GLN:O	1:A:163:GLN:HG2	1.99	0.63
1:B:31:LEU:HB2	1:B:38:PRO:HG3	1.79	0.62
1:D:254:LEU:HD13	1:D:305:ILE:HG22	1.81	0.62
1:D:316:ASN:HD21	1:D:322:GLU:H	1.48	0.62
2:K:10:LEU:HD12	2:K:10:LEU:H	1.64	0.61
1:B:158:ARG:NH1	1:B:159:GLU:OE2	2.34	0.60
1:D:159:GLU:HG3	1:D:159:GLU:O	2.01	0.60
1:B:192:LYS:HE3	1:B:196:ASP:OD2	2.01	0.59
1:D:166:SER:OG	1:D:168:ASP:OD2	2.17	0.59
1:B:308:LYS:NZ	1:B:308:LYS:HB3	2.19	0.58
1:C:27:LYS:NZ	1:C:39:GLU:OE2	2.31	0.58
1:C:103:LYS:HB3	1:D:235:LYS:HE3	1.85	0.58
1:C:69:ARG:NH1	1:C:345:ASN:O	2.37	0.57
1:A:192:LYS:HE3	1:A:196:ASP:OD2	2.03	0.57
1:B:23:GLN:NE2	1:B:49:GLU:HG3	2.19	0.57
1:C:192:LYS:HE3	1:C:196:ASP:OD1	2.04	0.57
2:F:13:LEU:O	2:F:17:VAL:HG23	2.04	0.57
1:A:166:SER:OG	1:A:168:ASP:OD1	2.18	0.57
1:B:180:LEU:O	1:B:184:GLN:HG3	2.05	0.56
2:K:14:ALA:O	2:K:17:VAL:HG12	2.06	0.56
1:B:163:GLN:OE1	1:B:163:GLN:N	2.30	0.56
1:A:63:GLU:OE1	1:C:132:ASP:OD2	2.23	0.56
1:D:180:LEU:O	1:D:184:GLN:HG3	2.05	0.56
1:D:254:LEU:O	1:D:258:LYS:HG3	2.05	0.56
1:C:198:ARG:HD2	2:H:13:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:O	1:A:184:GLN:HG3	2.05	0.55
1:C:261:GLU:HB2	1:C:269:ARG:HD3	1.88	0.55
1:D:192:LYS:HE3	1:D:196:ASP:OD1	2.07	0.54
1:A:329:THR:O	1:A:330:LEU:HD22	2.07	0.54
1:C:212:ASP:O	1:C:216:GLU:HG3	2.07	0.54
1:C:180:LEU:O	1:C:184:GLN:HG3	2.07	0.54
1:D:261:GLU:HB2	1:D:269:ARG:HD3	1.90	0.54
1:B:70:LYS:HD3	1:B:352:THR:O	2.08	0.54
1:C:1:MET:HG2	1:C:304:VAL:HG21	1.90	0.54
1:C:49:GLU:O	1:C:53:GLN:HG3	2.08	0.53
1:B:198:ARG:HD2	2:F:13:LEU:HD21	1.91	0.53
1:A:148:GLN:NE2	2:E:17:VAL:HG22	2.23	0.53
2:E:14:ALA:O	2:E:17:VAL:HG12	2.09	0.53
1:C:196:ASP:HB2	1:C:198:ARG:HG3	1.91	0.53
1:D:31:LEU:HB2	1:D:38:PRO:HG3	1.91	0.52
1:A:212:ASP:O	1:A:216:GLU:HG3	2.09	0.52
1:B:166:SER:OG	1:B:168:ASP:OD1	2.27	0.52
1:C:230:LEU:HB2	1:C:234:GLN:HB2	1.90	0.52
1:C:15:LYS:HG2	1:C:99:ILE:HG12	1.91	0.51
1:B:157:LEU:O	1:B:161:PHE:HB2	2.10	0.51
1:A:77:TYR:CZ	1:A:352:THR:HG21	2.46	0.50
1:D:189:LEU:HD21	1:D:338:LEU:HD12	1.93	0.50
1:C:261:GLU:OE2	1:C:308:LYS:NZ	2.45	0.50
1:B:269:ARG:NH1	3:B:404:HOH:O	2.44	0.50
1:C:140:MET:HE3	1:C:195:LEU:HD22	1.94	0.50
1:B:23:GLN:NE2	1:B:49:GLU:CG	2.75	0.49
1:B:89:GLU:OE2	1:B:89:GLU:N	2.40	0.49
1:A:77:TYR:HE1	1:A:352:THR:HG21	1.75	0.48
1:A:148:GLN:HE22	2:E:17:VAL:HG22	1.76	0.48
1:B:254:LEU:O	1:B:258:LYS:HG3	2.13	0.48
1:C:329:THR:O	1:C:330:LEU:HD12	2.13	0.48
1:C:202:LEU:HD11	2:H:10:LEU:HD21	1.94	0.48
1:C:275:SER:HB2	1:C:327:LEU:HD12	1.95	0.47
1:A:49:GLU:O	1:A:53:GLN:HG3	2.14	0.47
1:A:261:GLU:HB2	1:A:269:ARG:HD3	1.96	0.47
1:B:51:LEU:HD21	1:B:70:LYS:HG2	1.95	0.47
1:B:24:PRO:O	1:B:28:LYS:HE2	2.13	0.47
1:C:205:ARG:NH2	1:C:334:LYS:HE2	2.30	0.47
1:B:26:VAL:HG11	1:B:45:LEU:HD21	1.97	0.46
1:C:1:MET:HA	1:C:300:PHE:HE1	1.80	0.46
1:B:308:LYS:HB3	1:B:308:LYS:HZ1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LEU:HD23	1:C:327:LEU:HA	1.62	0.46
1:A:6:ARG:HB3	1:A:134:ARG:NH2	2.31	0.46
1:B:190:LEU:O	1:B:194:MET:HG3	2.15	0.46
1:C:98:GLU:OE2	1:C:101:SER:OG	2.16	0.45
1:D:189:LEU:HD21	1:D:338:LEU:HB2	1.98	0.45
1:B:26:VAL:O	1:B:30:VAL:HG23	2.16	0.45
1:B:230:LEU:HB2	1:B:234:GLN:HB2	1.98	0.45
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.82	0.45
1:A:330:LEU:CD2	1:A:330:LEU:N	2.80	0.44
1:C:128:LEU:HA	1:C:131:MET:HE3	1.98	0.44
1:B:259:GLN:HG3	1:B:260:ALA:N	2.30	0.44
1:C:254:LEU:O	1:C:258:LYS:HG3	2.17	0.44
1:D:316:ASN:ND2	1:D:322:GLU:H	2.14	0.44
1:D:348:ASP:HB3	1:D:351:VAL:HG22	2.00	0.44
1:A:329:THR:C	1:A:330:LEU:CD2	2.85	0.44
1:D:137:GLU:HA	1:D:140:MET:HE3	2.00	0.44
1:C:26:VAL:O	1:C:30:VAL:HG23	2.18	0.44
1:B:229:LEU:HG	1:B:230:LEU:HD23	2.01	0.43
1:C:355:ASP:HB3	1:C:358:ALA:HB2	1.99	0.43
1:C:41:TYR:CE1	1:C:359:LYS:HE3	2.54	0.43
1:D:107:HIS:HE1	1:D:165:TYR:O	2.02	0.43
1:C:124:LEU:O	1:C:128:LEU:HG	2.18	0.43
1:C:166:SER:HB3	1:C:168:ASP:OD1	2.19	0.42
1:D:258:LYS:HB3	1:D:258:LYS:HE2	1.84	0.42
1:A:41:TYR:CE1	1:A:359:LYS:HE3	2.55	0.42
1:C:83:PRO:HB2	1:C:88:GLN:HB3	2.01	0.42
1:D:32:LYS:NZ	1:D:89:GLU:OE2	2.39	0.42
1:B:45:LEU:HD23	1:B:357:PHE:HZ	1.85	0.41
1:A:23:GLN:HB2	1:A:24:PRO:HD3	2.02	0.41
1:A:308:LYS:HB3	1:A:308:LYS:HE3	1.87	0.41
1:C:137:GLU:O	1:C:137:GLU:HG2	2.21	0.41
1:D:189:LEU:CD2	1:D:338:LEU:HB2	2.51	0.41
1:C:140:MET:CE	1:C:195:LEU:HD22	2.49	0.41
1:D:22:PHE:CE1	1:D:48:LEU:HD23	2.55	0.41
1:B:49:GLU:O	1:B:53:GLN:HG3	2.21	0.41
1:D:259:GLN:O	1:D:263:GLN:HG3	2.21	0.41
1:B:199:LYS:HE2	1:B:199:LYS:HB2	1.89	0.41
1:B:23:GLN:HE21	1:B:49:GLU:HG3	1.86	0.41
1:A:164:ALA:HB2	1:A:170:SER:HA	2.03	0.41
1:A:330:LEU:HD22	1:A:330:LEU:N	2.31	0.40
1:C:59:PRO:HB2	1:C:61:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:VAL:HG12	1:C:215:LYS:HD2	2.02	0.40
1:A:128:LEU:HD23	1:A:131:MET:CE	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LYS:NZ	1:D:281:ASN:OD1[1_554]	1.54	0.66

## 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	356/361 (99%)	348 (98%)	8 (2%)	0	100	100
1	B	356/361 (99%)	350 (98%)	6 (2%)	0	100	100
1	C	357/361 (99%)	353 (99%)	4 (1%)	0	100	100
1	D	357/361 (99%)	350 (98%)	7 (2%)	0	100	100
2	E	9/18 (50%)	9 (100%)	0	0	100	100
2	F	9/18 (50%)	9 (100%)	0	0	100	100
2	H	9/18 (50%)	9 (100%)	0	0	100	100
2	K	9/18 (50%)	9 (100%)	0	0	100	100
All	All	1462/1516 (96%)	1437 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	302/304 (99%)	298 (99%)	4 (1%)	69	87
1	B	302/304 (99%)	297 (98%)	5 (2%)	60	82
1	C	304/304 (100%)	301 (99%)	3 (1%)	76	90
1	D	302/304 (99%)	298 (99%)	4 (1%)	69	87
2	E	9/16 (56%)	9 (100%)	0	100	100
2	F	9/16 (56%)	9 (100%)	0	100	100
2	H	9/16 (56%)	9 (100%)	0	100	100
2	K	9/16 (56%)	8 (89%)	1 (11%)	6	11
All	All	1246/1280 (97%)	1229 (99%)	17 (1%)	67	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	47	LYS
1	A	195	LEU
1	A	199	LYS
1	B	16	GLU
1	B	28	LYS
1	B	198	ARG
1	B	259	GLN
1	B	334	LYS
1	C	47	LYS
1	C	63	GLU
1	C	236	ASP
1	D	198	ARG
1	D	243	MET
1	D	328	ASP
1	D	340	LYS
2	K	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN

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Mol	Chain	Res	Type
1	A	177	ASN
1	B	255	HIS
1	C	281	ASN
1	C	295	GLN
1	D	107	HIS
1	D	186	GLN
1	D	316	ASN

### 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 monosaccharides 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
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	36:GLU	C	37:ASN	N	6.04



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	358/361 (99%)	-0.23	5 (1%) 75 77	26, 42, 66, 128	0
1	B	358/361 (99%)	-0.20	2 (0%) 89 90	29, 47, 73, 91	0
1	C	361/361 (100%)	-0.25	3 (0%) 86 87	26, 42, 68, 120	0
1	D	359/361 (99%)	-0.25	5 (1%) 75 77	31, 45, 73, 103	0
2	E	11/18 (61%)	0.81	1 (9%) 9 9	51, 70, 87, 103	0
2	F	11/18 (61%)	0.83	1 (9%) 9 9	53, 70, 85, 87	0
2	H	11/18 (61%)	2.07	5 (45%) 0 0	73, 82, 111, 114	0
2	K	11/18 (61%)	0.64	1 (9%) 9 9	61, 76, 92, 112	0
All	All	1480/1516 (97%)	-0.19	23 (1%) 72 74	26, 44, 76, 128	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	THR	7.9
2	H	18	SER	5.8
1	C	37	ASN	5.1
2	H	15	GLU	4.2
1	A	163	GLN	3.5
2	K	15	GLU	3.4
1	A	330	LEU	3.3
1	A	326	ALA	3.2
1	C	331	GLN	3.2
1	D	331	GLN	3.1
2	F	15	GLU	2.9
1	A	327	LEU	2.8
1	C	351	VAL	2.6
1	D	159	GLU	2.5
2	H	16	TRP	2.4
1	D	57	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	329	THR	2.3
2	H	11	LYS	2.2
1	D	330	LEU	2.1
2	H	9	ALA	2.1
1	B	361	VAL	2.1
1	B	50	LEU	2.1
2	E	8	GLU	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.