



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:34 AM UTC

PDB ID : 5CRU / pdb_00005cru
Title : Crystal structure of the Bro domain of HD-PTP
Authors : Lee, J.; Ku, B.; Kim, S.J.
Deposited on : 2015-07-23
Resolution : 2.40 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

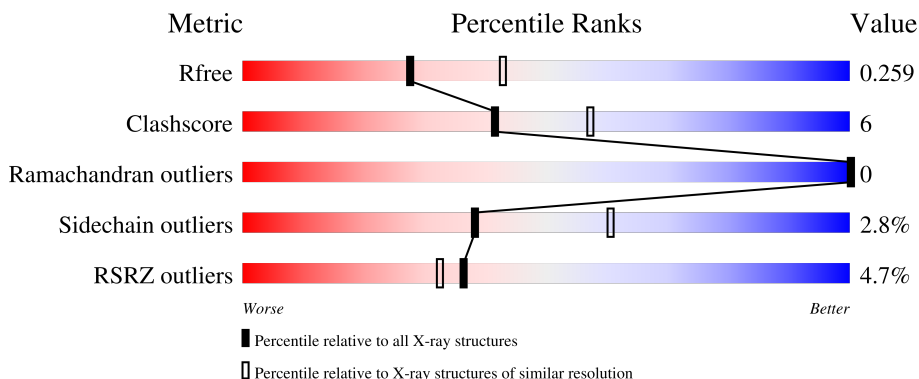
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	361	4% 85% 14% .
1	B	361	4% 86% 11% ..
1	C	361	4% 83% 15% .
1	D	361	7% 80% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11411 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	360	Total	C	N	O	S	0	1	0
			2853	1823	489	521	20			
1	B	357	Total	C	N	O	S	0	1	0
			2833	1811	485	518	19			
1	C	360	Total	C	N	O	S	0	1	0
			2853	1823	489	521	20			
1	D	357	Total	C	N	O	S	0	0	0
			2828	1806	485	518	19			

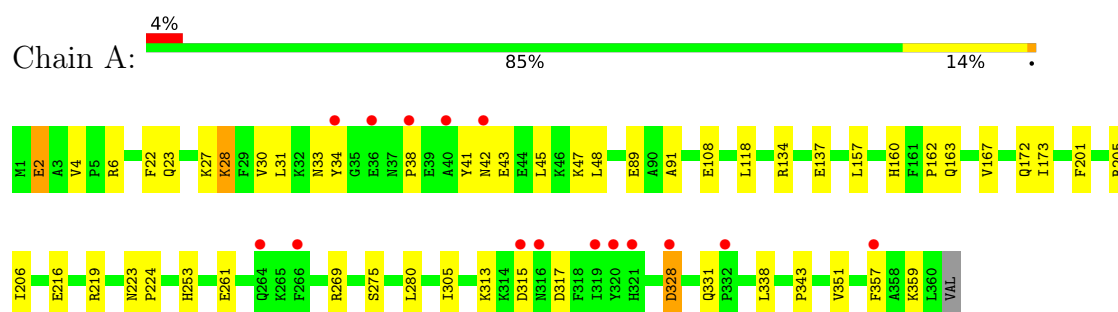
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	11	Total	O	0	0
			11	11		
2	C	13	Total	O	0	0
			13	13		
2	D	10	Total	O	0	0
			10	10		

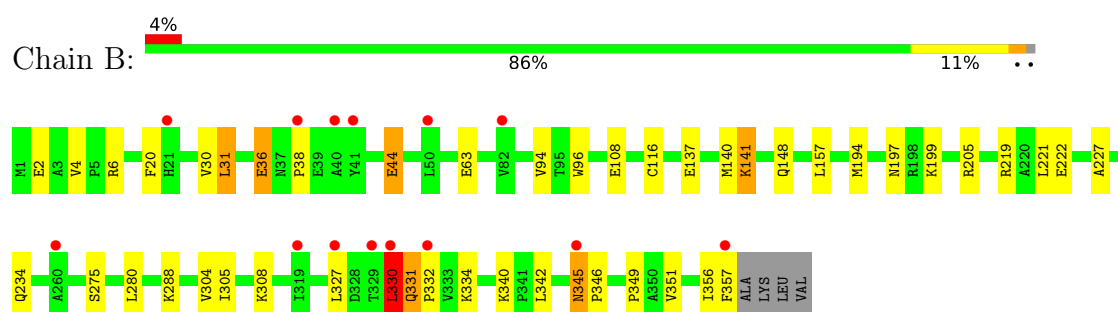
3 Residue-property plots [i](#)

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.

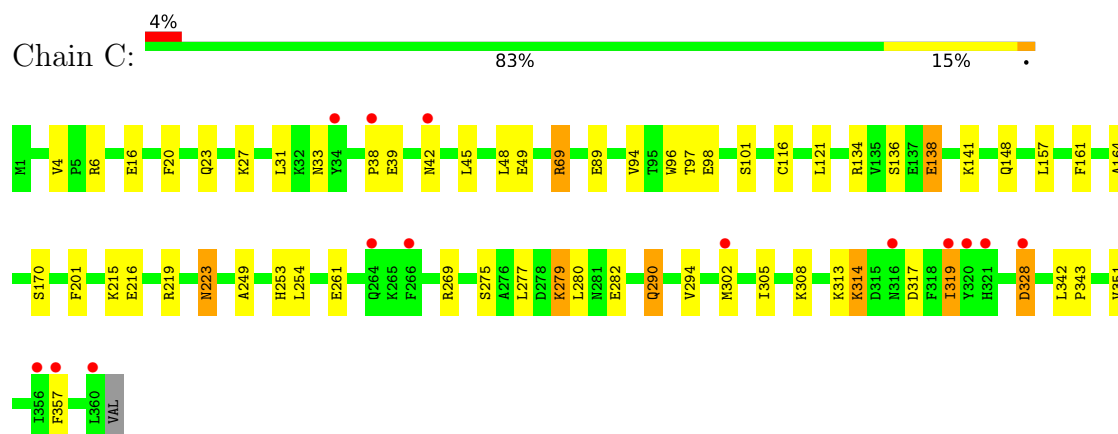
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 23



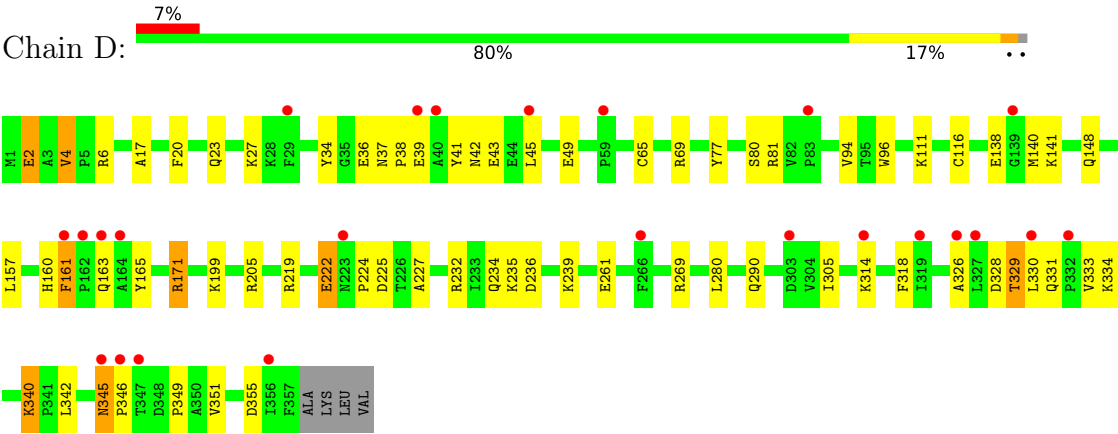
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 23



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.99Å 66.87Å 82.42Å 89.95° 89.94° 89.84°	Depositor
Resolution (Å)	30.98 – 2.40 30.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.98-2.40) 94.0 (30.98-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.36Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.220 , 0.259 0.223 , 0.259	Depositor DCC
R_{free} test set	2056 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,-h,l 0.000 for -k,h,l 0.458 for h,-k,-l 0.027 for -h,k,-l 0.026 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11411	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2583e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.34	0/2920	0.78	1/3943 (0.0%)
1	B	0.37	0/2898	0.87	5/3915 (0.1%)
1	C	0.40	0/2920	0.86	6/3943 (0.2%)
1	D	0.38	0/2890	0.89	9/3904 (0.2%)
All	All	0.37	0/11628	0.85	21/15705 (0.1%)

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
1	B	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	ILE	CB-CA-C	11.60	121.57	111.71
1	D	331	GLN	CA-C-N	9.14	129.71	119.92
1	D	331	GLN	C-N-CA	9.14	129.71	119.92
1	B	331	GLN	CA-C-N	8.23	128.16	119.85
1	B	331	GLN	C-N-CA	8.23	128.16	119.85
1	C	290	GLN	CA-CB-CG	8.06	130.23	114.10
1	B	345	ASN	CA-C-N	7.94	128.02	119.28
1	B	345	ASN	C-N-CA	7.94	128.02	119.28
1	C	319	ILE	N-CA-CB	-7.22	104.42	111.57
1	D	161	PHE	CA-C-N	6.45	126.03	119.19
1	D	161	PHE	C-N-CA	6.45	126.03	119.19
1	D	345	ASN	CA-C-N	6.39	126.31	119.28
1	D	345	ASN	C-N-CA	6.39	126.31	119.28
1	D	329	THR	N-CA-C	6.08	119.89	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	HIS	N-CA-C	-6.06	105.88	113.28
1	D	43	GLU	N-CA-C	-5.74	105.38	112.90
1	C	223	ASN	CA-C-N	5.59	125.69	119.32
1	C	223	ASN	C-N-CA	5.59	125.69	119.32
1	C	290	GLN	N-CA-CB	5.59	118.09	110.05
1	A	28	LYS	N-CA-C	-5.25	106.38	112.89
1	B	36	GLU	N-CA-C	5.18	121.83	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	330	LEU	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	2853	0	2869	34	1
1	B	2833	0	2846	38	0
1	C	2853	0	2869	37	1
1	D	2828	0	2835	52	0
2	A	10	0	0	1	0
2	B	11	0	0	1	0
2	C	13	0	0	1	0
2	D	10	0	0	0	0
All	All	11411	0	11419	145	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 6.

All (145) 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:B:199:LYS:HD2	1:B:199:LYS:H	1.28	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:NZ	1:A:42:ASN:OD1	2.02	0.92
1:D:219:ARG:NH1	1:D:222:GLU:OE2	2.06	0.88
1:C:27:LYS:NZ	1:C:42:ASN:OD1	2.11	0.83
1:C:33:ASN:OD1	1:D:205:ARG:NH1	2.14	0.80
1:C:27:LYS:NZ	1:C:38:PRO:O	2.16	0.79
1:D:4:VAL:O	1:D:6:ARG:NH2	2.19	0.76
1:C:98:GLU:OE1	1:C:101:SER:OG	2.05	0.75
1:A:48:LEU:HD22	1:A:357:PHE:HZ	1.53	0.74
1:D:138:GLU:OE1	1:D:141:LYS:NZ	2.21	0.74
1:B:4:VAL:O	1:B:6:ARG:NH2	2.21	0.74
1:B:194:MET:O	1:D:171:ARG:NH2	2.22	0.72
1:B:31:LEU:HD11	1:B:38:PRO:HD3	1.71	0.72
1:D:314:LYS:HZ2	1:D:318:PHE:HE2	1.39	0.71
1:B:219:ARG:NH1	1:B:222:GLU:OE1	2.24	0.71
1:A:33:ASN:OD1	1:B:205:ARG:NH1	2.26	0.68
1:C:27:LYS:HZ1	1:C:39:GLU:HA	1.59	0.67
1:C:290:GLN:HG3	1:C:294:VAL:HG11	1.77	0.67
1:A:280:LEU:HD22	1:A:305:ILE:HD12	1.80	0.64
1:A:216:GLU:OE2	1:A:219:ARG:NH1	2.30	0.64
1:B:63:GLU:HG2	1:D:328:ASP:O	1.98	0.64
1:A:261:GLU:HB2	1:A:269:ARG:HD2	1.80	0.63
1:D:65:CYS:O	1:D:69:ARG:HG3	1.98	0.63
1:B:356:ILE:HG22	1:B:357:PHE:HD1	1.64	0.62
1:D:157:LEU:O	1:D:161:PHE:HB2	1.99	0.62
1:D:148:GLN:HB3	1:D:342:LEU:HG	1.83	0.61
1:C:31:LEU:HB2	1:C:38:PRO:HD3	1.82	0.60
1:B:356:ILE:HG22	1:B:357:PHE:CD1	2.36	0.60
1:C:69:ARG:HH21	1:C:121:LEU:HD11	1.67	0.60
1:C:216:GLU:OE2	1:C:219:ARG:NH1	2.35	0.60
1:C:16:GLU:HG2	1:C:97:THR:HB	1.83	0.60
1:A:31:LEU:HB2	1:A:38:PRO:HD3	1.85	0.59
1:D:23:GLN:HB3	1:D:45:LEU:HD23	1.85	0.59
1:A:331:GLN:H	1:A:331:GLN:CD	2.10	0.58
1:A:30:VAL:HG23	1:A:34:TYR:HD2	1.69	0.57
1:B:148:GLN:HB3	1:B:342:LEU:HG	1.87	0.57
1:A:172:GLN:NE2	2:A:401:HOH:O	2.32	0.57
1:C:201:PHE:HE2	1:D:34:TYR:HE1	1.52	0.56
1:A:163:GLN:OE1	1:A:163:GLN:N	2.29	0.56
1:B:6:ARG:HH11	1:B:140:MET:HE2	1.69	0.56
1:B:197:ASN:CG	1:D:171:ARG:HH12	2.13	0.56
1:C:96:TRP:CG	1:C:116:CYS:HG	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:HG2	1:C:45:LEU:HB3	1.89	0.55
1:B:327:LEU:O	1:B:330:LEU:HD23	2.07	0.54
1:C:280:LEU:HD22	1:C:305:ILE:HD12	1.88	0.54
1:A:163:GLN:H	1:A:163:GLN:CD	2.14	0.53
1:A:313:LYS:NZ	1:A:317:ASP:OD2	2.40	0.53
1:D:77:TYR:O	1:D:80:SER:OG	2.26	0.53
1:A:4:VAL:O	1:A:6:ARG:NH2	2.41	0.53
1:B:108:GLU:OE2	2:B:401:HOH:O	2.19	0.53
1:A:359:LYS:HB3	1:D:224:PRO:HG3	1.91	0.53
1:A:2:GLU:H	1:A:2:GLU:CD	2.16	0.53
1:A:23:GLN:HG2	1:A:45:LEU:HB3	1.91	0.53
1:C:261:GLU:HB2	1:C:269:ARG:HD2	1.91	0.52
1:B:137:GLU:CD	1:D:219:ARG:HB3	2.34	0.52
1:A:43:GLU:OE2	1:D:235:LYS:NZ	2.22	0.52
1:B:96:TRP:CG	1:B:116:CYS:HG	2.27	0.52
1:D:163:GLN:OE1	1:D:165:TYR:CE2	2.62	0.52
1:C:4:VAL:O	1:C:6:ARG:NH2	2.43	0.51
1:D:280:LEU:HD22	1:D:305:ILE:HD12	1.93	0.51
1:C:223:ASN:ND2	2:C:401:HOH:O	2.45	0.50
1:B:304:VAL:O	1:B:308:LYS:HG3	2.11	0.50
1:A:91:ALA:HB1	1:A:108:GLU:HG2	1.93	0.50
1:D:205:ARG:NH2	1:D:334:LYS:HG3	2.26	0.50
1:A:253:HIS:ND1	1:A:275:SER:OG	2.41	0.50
1:A:343:PRO:HG2	1:B:349:PRO:HD3	1.94	0.50
1:C:157:LEU:HD23	1:C:161:PHE:HB2	1.93	0.50
1:D:326:ALA:O	1:D:329:THR:OG1	2.29	0.49
1:A:22:PHE:CE1	1:A:48:LEU:HD23	2.47	0.49
1:D:314:LYS:NZ	1:D:318:PHE:HE2	2.07	0.49
1:D:6:ARG:HH11	1:D:140:MET:HE2	1.76	0.49
1:A:160:HIS:C	1:A:162:PRO:HD3	2.39	0.48
1:D:96:TRP:CG	1:D:116:CYS:HG	2.30	0.48
1:D:330:LEU:HD12	1:D:330:LEU:HA	1.69	0.47
1:D:314:LYS:HA	1:D:314:LYS:HD2	1.58	0.47
1:A:48:LEU:HD22	1:A:357:PHE:CZ	2.41	0.47
1:B:30:VAL:HG13	1:B:31:LEU:HD23	1.97	0.47
1:C:164:ALA:HB2	1:C:170:SER:HA	1.97	0.46
1:A:167:VAL:O	1:A:173:ILE:HD12	2.15	0.46
1:B:280:LEU:HD22	1:B:305:ILE:HD12	1.98	0.46
1:C:148:GLN:HB3	1:C:342:LEU:HG	1.98	0.46
1:B:334:LYS:HE3	1:B:334:LYS:HB2	1.50	0.46
1:A:6:ARG:HB3	1:A:134:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:GLU:H	1:D:2:GLU:CD	2.20	0.46
1:B:31:LEU:HD22	1:B:36:GLU:HB2	1.97	0.45
1:B:345:ASN:HA	1:B:346:PRO:HD3	1.70	0.45
1:C:343:PRO:HG2	1:D:349:PRO:HD3	1.97	0.45
1:D:232:ARG:HG3	1:D:232:ARG:HH11	1.82	0.45
1:A:118:LEU:HD23	1:A:157:LEU:HG	1.99	0.45
1:B:141:LYS:HZ1	1:D:219:ARG:NH2	2.14	0.45
1:C:249:ALA:HB1	1:C:279:LYS:HE2	1.99	0.45
1:D:39:GLU:HA	1:D:42:ASN:OD1	2.17	0.45
1:D:314:LYS:CE	1:D:318:PHE:HE2	2.29	0.45
1:B:199:LYS:HD2	1:B:199:LYS:N	2.09	0.45
1:B:331:GLN:HA	1:B:332:PRO:HD3	1.67	0.45
1:D:261:GLU:HB2	1:D:269:ARG:HD2	1.99	0.45
1:A:261:GLU:HB2	1:A:269:ARG:CD	2.46	0.44
1:C:69:ARG:NH2	1:C:121:LEU:HD11	2.32	0.44
1:C:313:LYS:NZ	1:C:317:ASP:OD2	2.40	0.44
1:B:330:LEU:HD12	1:B:332:PRO:HD3	1.98	0.44
1:D:111:LYS:NZ	1:D:163:GLN:HE22	2.15	0.44
1:B:31:LEU:HA	1:B:36:GLU:H	1.82	0.44
1:D:219:ARG:HD3	1:D:219:ARG:HA	1.23	0.44
1:D:81:ARG:NH1	1:D:355:ASP:OD2	2.50	0.44
1:D:239:LYS:HG3	1:D:290:GLN:NE2	2.32	0.44
1:C:277:LEU:HD11	1:C:302:MET:HE2	2.00	0.44
1:C:253:HIS:ND1	1:C:275:SER:OG	2.43	0.43
1:C:136:SER:OG	1:C:138:GLU:HG2	2.18	0.43
1:D:27:LYS:HE3	1:D:45:LEU:CD2	2.48	0.43
1:B:327:LEU:O	1:B:330:LEU:HB3	2.18	0.43
1:C:314:LYS:HB3	1:C:314:LYS:HE2	1.49	0.43
1:D:345:ASN:HA	1:D:346:PRO:HD3	1.78	0.43
1:A:41:TYR:O	1:A:45:LEU:HD13	2.18	0.43
1:B:2:GLU:H	1:B:2:GLU:HG2	1.35	0.43
1:C:277:LEU:HA	1:C:277:LEU:HD12	1.81	0.43
1:D:340:LYS:HA	1:D:340:LYS:HD2	1.63	0.43
1:C:254:LEU:HD11	1:C:308:LYS:HD2	2.01	0.42
1:C:138:GLU:HG2	1:C:138:GLU:H	1.42	0.42
1:A:328:ASP:OD1	1:A:328:ASP:N	2.48	0.42
1:D:23:GLN:NE2	1:D:49:GLU:OE1	2.53	0.42
1:B:44:GLU:HB2	1:B:357:PHE:CE1	2.55	0.42
1:B:199:LYS:NZ	1:D:225:ASP:OD2	2.47	0.42
1:A:223:ASN:HA	1:A:224:PRO:HD2	1.83	0.41
1:A:206:ILE:HG12	1:A:338:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:PHE:CD1	1:D:94:VAL:HG22	2.55	0.41
1:D:227:ALA:HA	1:D:234:GLN:HG3	2.02	0.41
1:C:48:LEU:HD22	1:C:357:PHE:HZ	1.86	0.41
1:D:161:PHE:HD2	1:D:163:GLN:OE1	2.04	0.41
1:B:219:ARG:HD3	1:B:219:ARG:HA	1.31	0.41
1:B:2:GLU:HB3	1:D:171:ARG:HE	1.86	0.41
1:B:197:ASN:CB	1:D:171:ARG:HH12	2.33	0.41
1:C:6:ARG:HB3	1:C:134:ARG:NH2	2.36	0.41
1:D:37:ASN:HA	1:D:38:PRO:HD2	1.96	0.41
1:A:201:PHE:O	1:A:205:ARG:HG3	2.21	0.41
1:C:328:ASP:OD1	1:C:328:ASP:N	2.54	0.41
1:A:269:ARG:NH1	1:A:315:ASP:OD2	2.49	0.41
1:B:275:SER:HB2	1:B:327:LEU:HD13	2.02	0.41
1:C:48:LEU:HD22	1:C:357:PHE:CZ	2.57	0.41
1:C:201:PHE:CE2	1:D:34:TYR:HE1	2.36	0.41
1:D:36:GLU:OE1	1:D:41:TYR:CE1	2.74	0.41
1:D:17:ALA:HB2	1:D:96:TRP:CH2	2.56	0.40
1:D:236:ASP:O	1:D:239:LYS:HG2	2.21	0.40
1:C:20:PHE:CD1	1:C:94:VAL:HG22	2.56	0.40
1:B:227:ALA:HA	1:B:234:GLN:HG3	2.03	0.40
1:B:20:PHE:CD1	1:B:94:VAL:HG22	2.56	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:A:137:GLU:OE2	1:C:215:LYS:NZ[1_564]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/361 (99%)	354 (99%)	5 (1%)	0	100	100
1	B	356/361 (99%)	348 (98%)	8 (2%)	0	100	100
1	C	359/361 (99%)	354 (99%)	5 (1%)	0	100	100
1	D	355/361 (98%)	350 (99%)	5 (1%)	0	100	100
All	All	1429/1444 (99%)	1406 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	304/304 (100%)	298 (98%)	6 (2%)	48	70
1	B	302/304 (99%)	292 (97%)	10 (3%)	33	55
1	C	304/304 (100%)	293 (96%)	11 (4%)	31	52
1	D	301/304 (99%)	293 (97%)	8 (3%)	39	62
All	All	1211/1216 (100%)	1176 (97%)	35 (3%)	38	60

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	28	LYS
1	A	47	LYS
1	A	89	GLU
1	A	328	ASP
1	A	351	VAL
1	B	31	LEU
1	B	44	GLU
1	B	141	LYS
1	B	157	LEU
1	B	221[A]	LEU
1	B	221[B]	LEU
1	B	288	LYS

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Mol	Chain	Res	Type
1	B	330	LEU
1	B	340	LYS
1	B	351	VAL
1	C	49	GLU
1	C	69	ARG
1	C	89	GLU
1	C	138	GLU
1	C	141	LYS
1	C	279	LYS
1	C	282	GLU
1	C	314	LYS
1	C	319	ILE
1	C	328	ASP
1	C	351	VAL
1	D	2	GLU
1	D	4	VAL
1	D	171	ARG
1	D	199	LYS
1	D	222	GLU
1	D	333	VAL
1	D	340	LYS
1	D	351	VAL

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	209	GLN
1	A	316	ASN
1	B	316	ASN
1	C	37	ASN
1	C	223	ASN
1	D	33	ASN
1	D	163	GLN
1	D	290	GLN

5.3.3 RNA ⓘ

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	360/361 (99%)	0.37	15 (4%)	40 36	25, 44, 74, 100	1 (0%)
1	B	357/361 (98%)	0.46	14 (3%)	43 39	24, 45, 84, 101	1 (0%)
1	C	360/361 (99%)	0.39	14 (3%)	43 39	25, 44, 75, 101	1 (0%)
1	D	357/361 (98%)	0.47	24 (6%)	24 20	25, 45, 80, 105	0
All	All	1434/1444 (99%)	0.42	67 (4%)	36 32	24, 45, 77, 105	3 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	TYR	6.0
1	B	330	LEU	3.9
1	D	40	ALA	3.8
1	B	40	ALA	3.8
1	A	38	PRO	3.3
1	C	38	PRO	3.3
1	A	319	ILE	3.3
1	B	357	PHE	3.2
1	D	330	LEU	3.1
1	C	328	ASP	2.9
1	D	314	LYS	2.9
1	D	161	PHE	2.9
1	D	39	GLU	2.9
1	D	346	PRO	2.8
1	C	356	ILE	2.7
1	D	345	ASN	2.7
1	B	21	HIS	2.7
1	A	320	TYR	2.7
1	D	139	GLY	2.6
1	D	303	ASP	2.6
1	C	302	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	2.5
1	A	34	TYR	2.5
1	D	332	PRO	2.5
1	A	315	ASP	2.5
1	C	357	PHE	2.5
1	B	329	THR	2.5
1	B	332	PRO	2.5
1	C	264	GLN	2.5
1	B	41	TYR	2.4
1	C	360	LEU	2.4
1	A	264	GLN	2.4
1	A	316	ASN	2.4
1	A	36	GLU	2.4
1	B	50	LEU	2.4
1	D	266	PHE	2.4
1	D	29	PHE	2.4
1	D	45	LEU	2.3
1	A	357	PHE	2.3
1	D	83	PRO	2.3
1	B	327	LEU	2.3
1	D	163	GLN	2.3
1	D	347	THR	2.2
1	C	319	ILE	2.2
1	A	266	PHE	2.2
1	B	345	ASN	2.2
1	C	321	HIS	2.2
1	B	38	PRO	2.2
1	D	59	PRO	2.2
1	D	327	LEU	2.2
1	C	42	ASN	2.2
1	D	223	ASN	2.2
1	A	332	PRO	2.2
1	D	162	PRO	2.1
1	A	321	HIS	2.1
1	B	82	VAL	2.1
1	B	319	ILE	2.1
1	D	319	ILE	2.1
1	D	356	ILE	2.1
1	D	326	ALA	2.1
1	C	266	PHE	2.0
1	D	164	ALA	2.0
1	C	316	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	328	ASP	2.0
1	C	34	TYR	2.0
1	B	260	ALA	2.0
1	A	42	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.