



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:41 AM UTC

PDB ID : 5YKD / pdb_00005ykd
Title : Crystal structure of dihydropyrimidinase from *Pseudomonas aeruginosa* PAO1 at 2.17 angstrom resolution
Authors : Huang, Y.H.; Huang, C.Y.
Deposited on : 2017-10-14
Resolution : 2.17 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

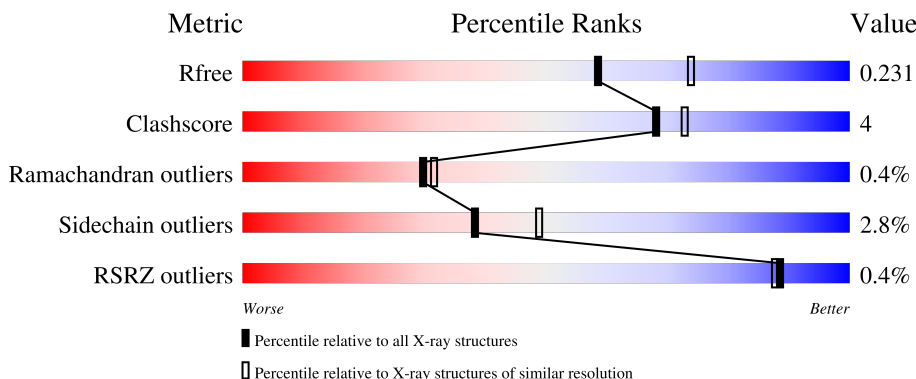
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	479	89%10%
1	B	479	90%9%
1	C	479	88%11%
1	D	479	88%10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15005 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 D-hydantoinase/dihydropyrimidinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3671	2311	659	685	16			
1	B	478	Total	C	N	O	S	0	0	0
			3671	2311	659	685	16			
1	C	478	Total	C	N	O	S	0	0	0
			3671	2311	659	685	16			
1	D	478	Total	C	N	O	S	0	0	0
			3671	2311	659	685	16			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

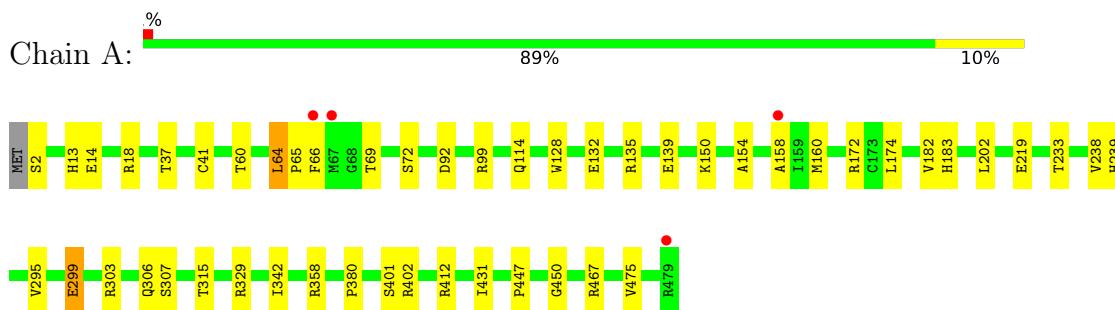
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total	O	0	0
			84	84		
3	B	102	Total	O	0	0
			102	102		
3	C	69	Total	O	0	0
			69	69		
3	D	58	Total	O	0	0
			58	58		

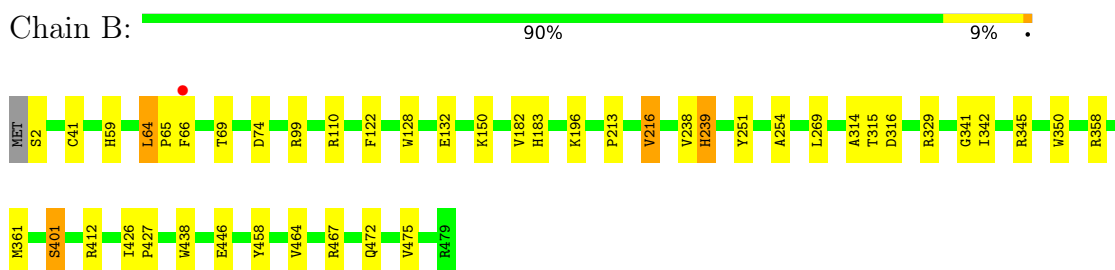
3 Residue-property plots

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.

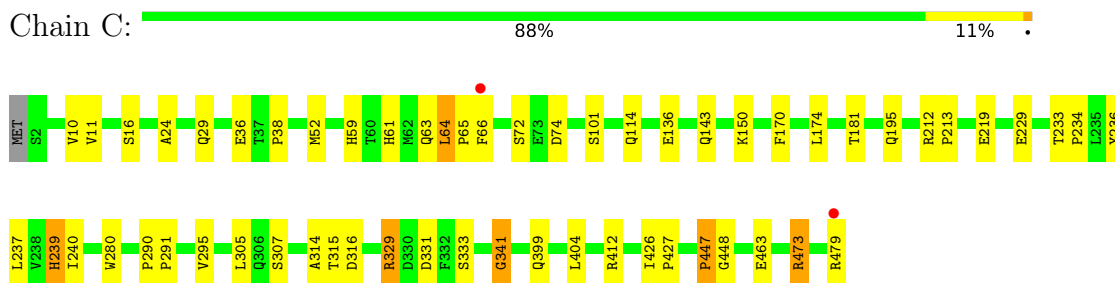
- Molecule 1: D-hydantoinase/dihydropyrimidinase



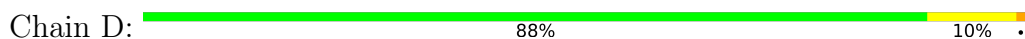
- Molecule 1: D-hydantoinase/dihydropyrimidinase

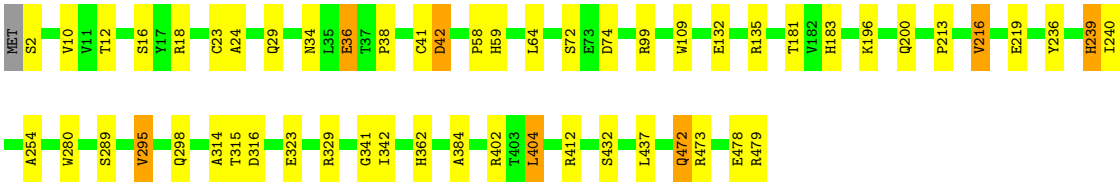


- Molecule 1: D-hydantoinase/dihydropyrimidinase



- Molecule 1: D-hydantoinase/dihydropyrimidinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.91Å 155.70Å 235.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.17 30.00 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.17) 99.8 (30.00-2.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.17Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.176 , 0.231 0.182 , 0.231	Depositor DCC
R_{free} test set	5323 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15005	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, ZN

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	1.11	3/3750 (0.1%)	1.02	4/5099 (0.1%)
1	B	1.07	4/3750 (0.1%)	1.01	5/5099 (0.1%)
1	C	1.05	4/3750 (0.1%)	1.01	2/5099 (0.0%)
1	D	1.03	1/3750 (0.0%)	0.99	3/5099 (0.1%)
All	All	1.07	12/15000 (0.1%)	1.01	14/20396 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ALA	CA-C	11.91	1.58	1.52
1	B	345	ARG	N-CA	6.27	1.53	1.46
1	A	172	ARG	N-CA	-6.02	1.39	1.46
1	C	305	LEU	C-O	-5.97	1.17	1.24
1	B	401	SER	C-O	-5.93	1.16	1.23
1	C	229	GLU	C-O	-5.70	1.17	1.24
1	B	438	TRP	CA-C	-5.54	1.46	1.52
1	D	289	SER	C-O	-5.43	1.18	1.25
1	C	213	PRO	CA-C	5.29	1.57	1.52
1	C	447	PRO	N-CA	-5.13	1.41	1.47
1	B	269	LEU	C-O	-5.09	1.17	1.24
1	A	431	ILE	N-CA	-5.05	1.40	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	TYR	CA-C-N	-6.47	111.75	119.84
1	B	458	TYR	C-N-CA	-6.47	111.75	119.84
1	A	295	VAL	CB-CA-C	-6.28	103.81	112.04
1	A	295	VAL	N-CA-C	6.12	117.59	110.62
1	B	358	ARG	N-CA-C	5.43	117.20	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	PHE	N-CA-C	-5.25	105.64	111.36
1	B	475	VAL	CB-CA-C	5.14	117.83	110.33
1	D	384	ALA	CA-C-N	-5.14	116.58	122.95
1	D	384	ALA	C-N-CA	-5.14	116.58	122.95
1	B	251	TYR	N-CA-C	-5.12	105.70	111.28
1	A	37	THR	CA-C-N	-5.07	114.50	119.92
1	A	37	THR	C-N-CA	-5.07	114.50	119.92
1	C	295	VAL	N-CA-C	5.05	117.36	111.05
1	D	295	VAL	N-CA-C	5.03	118.11	111.17

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	3671	0	3556	29	0
1	B	3671	0	3556	22	0
1	C	3671	0	3554	30	1
1	D	3671	0	3556	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	84	0	0	3	0
3	B	102	0	0	1	0
3	C	69	0	0	0	0
3	D	58	0	0	0	0
All	All	15005	0	14222	103	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 4.

All (103) 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:2:SER:CB	1:A:41:CYS:SG	2.48	1.01
1:A:2:SER:HB2	1:A:41:CYS:SG	2.01	0.99
1:D:2:SER:HG	1:D:41:CYS:HG	0.85	0.81
1:A:2:SER:HB3	1:A:41:CYS:SG	2.21	0.78
1:B:2:SER:CB	1:B:41:CYS:HG	1.97	0.77
1:D:2:SER:OG	1:D:41:CYS:SG	2.18	0.75
1:A:64:LEU:HD13	1:A:66:PHE:HB2	1.68	0.74
1:D:72:SER:O	1:D:412:ARG:NH1	2.18	0.73
1:B:2:SER:CB	1:B:41:CYS:SG	2.76	0.73
1:A:450:GLY:O	3:A:601:HOH:O	2.14	0.65
1:B:467:ARG:NH2	3:B:601:HOH:O	2.30	0.64
1:C:64:LEU:HD13	1:C:66:PHE:HB2	1.82	0.61
1:A:303:ARG:HA	1:A:306:GLN:HE21	1.65	0.60
1:A:299:GLU:OE1	1:A:358:ARG:NH2	2.35	0.59
1:B:426:ILE:HB	1:B:427:PRO:HD2	1.87	0.57
1:D:2:SER:CB	1:D:41:CYS:SG	2.93	0.57
3:A:601:HOH:O	1:C:114:GLN:NE2	2.36	0.57
1:A:2:SER:HB2	1:A:41:CYS:HG	1.71	0.56
1:A:315:THR:HG21	1:A:342:ILE:HA	1.87	0.56
1:C:63:GLN:OE1	1:C:74:ASP:HB2	2.08	0.53
1:B:2:SER:HB3	1:B:41:CYS:SG	2.49	0.53
1:D:74:ASP:OD2	1:D:412:ARG:NH2	2.42	0.53
1:B:64:LEU:HD13	1:B:66:PHE:HB2	1.90	0.52
1:C:315:THR:HG21	1:C:341:GLY:C	2.34	0.52
1:C:331:ASP:OD1	1:C:333:SER:OG	2.27	0.51
1:D:42:ASP:N	1:D:42:ASP:OD1	2.42	0.51
1:B:59:HIS:HB3	1:B:314:ALA:HB1	1.92	0.51
1:D:432:SER:HB3	1:D:437:LEU:HD12	1.92	0.51
1:D:181:THR:HA	1:D:236:TYR:O	2.10	0.51
1:D:295:VAL:HA	1:D:298:GLN:OE1	2.11	0.51
1:A:65:PRO:HA	1:A:69:THR:O	2.12	0.50
1:A:13:HIS:CD2	1:A:14:GLU:HG3	2.46	0.50
1:B:64:LEU:HD22	1:B:65:PRO:O	2.12	0.50
1:A:72:SER:O	1:A:412:ARG:HD2	2.12	0.50
1:D:315:THR:HG21	1:D:342:ILE:HA	1.93	0.50
1:C:426:ILE:HB	1:C:427:PRO:HD2	1.94	0.49
1:B:99:ARG:H	1:B:128:TRP:CG	2.30	0.49
1:D:280:TRP:CZ2	1:D:329:ARG:HA	2.47	0.49
1:A:64:LEU:HD13	1:A:66:PHE:CB	2.41	0.49
1:C:233:THR:HB	1:C:234:PRO:HD2	1.95	0.49
1:C:11:VAL:HB	1:C:52:MET:HG2	1.95	0.48
1:C:174:LEU:HB2	1:C:233:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:VAL:O	1:B:238:VAL:HG22	2.14	0.48
1:C:473:ARG:HH11	1:C:473:ARG:HG3	1.79	0.48
1:C:101:SER:OG	1:C:136:GLU:OE2	2.27	0.47
1:C:195:GLN:NE2	1:C:195:GLN:HA	2.28	0.47
1:C:10:VAL:O	1:C:16:SER:HA	2.13	0.47
1:C:219:GLU:CD	1:C:219:GLU:C	2.83	0.47
1:D:219:GLU:CD	1:D:219:GLU:C	2.81	0.47
1:D:2:SER:HA	1:D:23:CYS:O	2.14	0.47
1:A:239:HIS:O	1:A:239:HIS:CD2	2.68	0.47
1:A:467:ARG:NH2	3:A:603:HOH:O	2.36	0.47
1:A:174:LEU:HB2	1:A:233:THR:HG22	1.97	0.46
1:B:315:THR:HG21	1:B:342:ILE:HA	1.98	0.46
1:C:61:HIS:CD2	1:C:316:ASP:OD1	2.68	0.46
1:A:182:VAL:O	1:A:238:VAL:HG22	2.15	0.46
1:B:65:PRO:HA	1:B:69:THR:O	2.15	0.46
1:A:307:SER:HB3	1:B:254:ALA:HA	1.96	0.46
1:D:472:GLN:CA	1:D:472:GLN:HE21	2.28	0.46
1:A:447:PRO:HB2	1:C:447:PRO:HB2	1.98	0.45
1:A:132:GLU:HA	1:A:132:GLU:OE1	2.15	0.45
1:A:135:ARG:NH1	1:A:139:GLU:OE1	2.46	0.45
1:C:72:SER:O	1:C:412:ARG:HD2	2.16	0.45
1:B:213:PRO:O	1:B:216:VAL:HB	2.17	0.44
1:D:24:ALA:HB3	1:D:29:GLN:HG3	1.98	0.44
1:B:183:HIS:CD2	1:B:183:HIS:C	2.95	0.44
1:C:280:TRP:CZ2	1:C:329:ARG:HA	2.53	0.44
1:D:10:VAL:O	1:D:16:SER:HA	2.18	0.44
1:D:183:HIS:CD2	1:D:183:HIS:C	2.96	0.43
1:D:58:PRO:HD2	1:D:314:ALA:HB2	2.00	0.43
1:C:239:HIS:CE1	1:C:290:PRO:HD3	2.54	0.43
1:C:24:ALA:HB3	1:C:29:GLN:HG3	2.00	0.43
1:C:307:SER:HB3	1:D:254:ALA:HA	2.00	0.43
1:A:154:ALA:O	1:A:160:MET:HB2	2.19	0.43
1:D:132:GLU:OE2	1:D:135:ARG:NH2	2.38	0.43
1:C:64:LEU:HD13	1:C:66:PHE:CB	2.47	0.42
1:D:12:THR:O	1:D:362:HIS:HD2	2.02	0.42
1:B:2:SER:HB3	1:B:41:CYS:HA	2.01	0.42
1:A:114:GLN:HB3	1:C:448:GLY:O	2.20	0.42
1:A:132:GLU:OE2	1:A:135:ARG:NH2	2.47	0.42
1:B:59:HIS:CD2	1:B:316:ASP:HA	2.55	0.42
1:C:473:ARG:HH11	1:C:473:ARG:CG	2.32	0.42
1:D:59:HIS:CD2	1:D:316:ASP:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:HIS:O	1:D:239:HIS:CD2	2.72	0.42
1:D:2:SER:HG	1:D:41:CYS:CB	2.25	0.42
1:C:237:LEU:HB3	1:C:240:ILE:HD11	2.02	0.42
1:C:212:ARG:HG3	1:C:291:PRO:HD3	2.02	0.42
1:B:110:ARG:HD2	1:B:122:PHE:HE2	1.85	0.42
1:C:64:LEU:HD22	1:C:65:PRO:O	2.20	0.41
1:A:60:THR:O	1:A:92:ASP:HA	2.19	0.41
1:A:219:GLU:CD	1:A:219:GLU:C	2.88	0.41
1:A:303:ARG:HB3	1:B:254:ALA:O	2.21	0.41
1:B:239:HIS:O	1:B:239:HIS:CD2	2.73	0.41
1:D:213:PRO:O	1:D:216:VAL:HB	2.20	0.41
1:B:350:TRP:CH2	1:B:361:MET:HG2	2.55	0.41
1:D:36:GLU:O	1:D:38:PRO:HD3	2.20	0.41
1:A:183:HIS:CD2	1:A:183:HIS:C	2.98	0.41
1:C:36:GLU:O	1:C:38:PRO:HD3	2.20	0.41
1:C:181:THR:HA	1:C:236:TYR:O	2.20	0.41
1:D:402:ARG:CZ	1:D:404:LEU:HD22	2.51	0.41
1:C:59:HIS:HB3	1:C:314:ALA:HB1	2.02	0.41
1:A:99:ARG:H	1:A:128:TRP:CG	2.39	0.40
1:B:74:ASP:C	1:B:74:ASP:OD1	2.65	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:399:GLN:OE1	1:C:399:GLN:OE1[3_455]	2.13	0.07

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	475/479 (99%)	458 (96%)	17 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	475/479 (99%)	453 (95%)	20 (4%)	2 (0%)	30	31
1	C	475/479 (99%)	455 (96%)	18 (4%)	2 (0%)	30	31
1	D	475/479 (99%)	457 (96%)	15 (3%)	3 (1%)	21	20
All	All	1900/1916 (99%)	1823 (96%)	70 (4%)	7 (0%)	30	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	239	HIS
1	C	341	GLY
1	B	341	GLY
1	D	34	ASN
1	D	341	GLY
1	C	239	HIS
1	D	239	HIS

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	375/376 (100%)	366 (98%)	9 (2%)	43	55
1	B	375/376 (100%)	365 (97%)	10 (3%)	39	50
1	C	375/376 (100%)	368 (98%)	7 (2%)	50	63
1	D	375/376 (100%)	359 (96%)	16 (4%)	26	32
All	All	1500/1504 (100%)	1458 (97%)	42 (3%)	38	49

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	64	LEU
1	A	202	LEU
1	A	299	GLU

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Mol	Chain	Res	Type
1	A	329	ARG
1	A	380	PRO
1	A	401	SER
1	A	402	ARG
1	A	475	VAL
1	B	64	LEU
1	B	132	GLU
1	B	196	LYS
1	B	216	VAL
1	B	329	ARG
1	B	401	SER
1	B	412	ARG
1	B	446	GLU
1	B	464	VAL
1	B	472	GLN
1	C	64	LEU
1	C	143	GLN
1	C	329	ARG
1	C	404	LEU
1	C	463	GLU
1	C	473	ARG
1	C	479	ARG
1	D	18	ARG
1	D	36	GLU
1	D	42	ASP
1	D	64	LEU
1	D	99	ARG
1	D	109	TRP
1	D	196	LYS
1	D	200	GLN
1	D	216	VAL
1	D	240	ILE
1	D	323	GLU
1	D	404	LEU
1	D	472	GLN
1	D	473	ARG
1	D	478	GLU
1	D	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	239	HIS
1	A	306	GLN
1	A	399	GLN
1	B	143	GLN
1	B	239	HIS
1	B	306	GLN
1	B	411	GLN
1	C	114	GLN
1	C	144	HIS
1	C	157	ASN
1	C	183	HIS
1	C	195	GLN
1	C	411	GLN
1	D	192	HIS
1	D	239	HIS
1	D	306	GLN
1	D	433	GLN
1	D	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	A	150	1,2	10,11,12	1.93	1 (10%)	6,12,14	2.26	1 (16%)
1	KCX	C	150	1,2	10,11,12	1.80	1 (10%)	6,12,14	1.49	1 (16%)
1	KCX	B	150	1,2	10,11,12	0.74	0	6,12,14	1.11	1 (16%)
1	KCX	D	150	1,2	10,11,12	0.66	0	6,12,14	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	150	1,2	-	0/9/10/12	-
1	KCX	C	150	1,2	-	0/9/10/12	-
1	KCX	B	150	1,2	-	0/9/10/12	-
1	KCX	D	150	1,2	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	KCX	OQ1-CX	5.14	1.31	1.21
1	C	150	KCX	OQ1-CX	5.10	1.31	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	KCX	OQ1-CX-NZ	-5.38	116.75	124.92
1	C	150	KCX	OQ1-CX-NZ	-3.10	120.21	124.92
1	B	150	KCX	CE-NZ-CX	2.21	125.72	121.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	477/479 (99%)	-0.36	4 (0%) 82 82	26, 35, 54, 75	0
1	B	477/479 (99%)	-0.34	1 (0%) 91 90	27, 36, 56, 76	0
1	C	477/479 (99%)	-0.32	2 (0%) 88 88	29, 37, 57, 87	0
1	D	477/479 (99%)	-0.23	0 100 100	30, 39, 60, 85	0
All	All	1908/1916 (99%)	-0.31	7 (0%) 88 88	26, 37, 57, 87	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	PHE	3.8
1	C	479	ARG	2.9
1	C	66	PHE	2.6
1	A	67	MET	2.2
1	A	158	ALA	2.2
1	B	66	PHE	2.2
1	A	479	ARG	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	B	150	12/13	0.96	0.06	26,28,31,32	0
1	KCX	C	150	12/13	0.97	0.05	28,31,36,37	0
1	KCX	D	150	12/13	0.97	0.06	27,30,34,35	0
1	KCX	A	150	12/13	0.98	0.05	27,28,30,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	501	1/1	0.99	0.04	40,40,40,40	0
2	ZN	A	502	1/1	0.99	0.02	33,33,33,33	0
2	ZN	B	501	1/1	0.99	0.02	41,41,41,41	0
2	ZN	B	502	1/1	0.99	0.02	35,35,35,35	0
2	ZN	C	501	1/1	0.99	0.05	41,41,41,41	0
2	ZN	C	502	1/1	0.99	0.03	34,34,34,34	0
2	ZN	D	501	1/1	0.99	0.02	38,38,38,38	0
2	ZN	D	502	1/1	0.99	0.02	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.