



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:52 AM GMT

PDB ID : 2FTY  
Title : Crystal structure of dihydropyrimidinase from *Saccharomyces kluyveri*  
Authors : Dobritsch, D.; Lohkamp, B.  
Deposited on : 2006-01-25  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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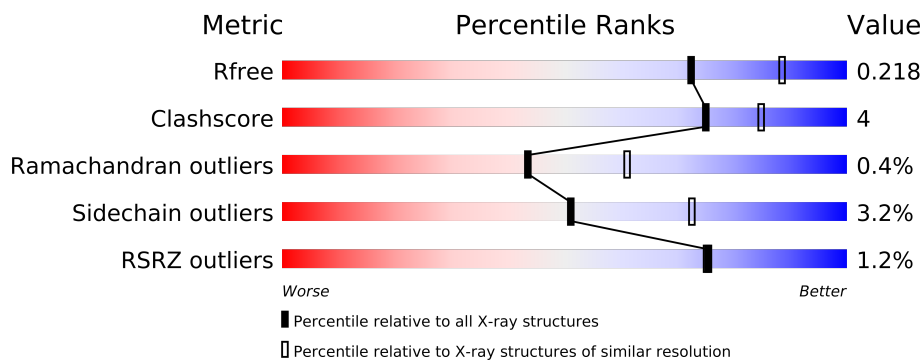
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	559	
1	B	559	
1	C	559	
1	D	559	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17311 atoms, of which 0 are hydrogen and 0 are deuterium.

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 dihydropyrimidinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	2	0
			4164	2646	680	811	27			
1	B	532	Total	C	N	O	S	0	3	0
			4169	2651	680	811	27			
1	C	531	Total	C	N	O	S	0	0	0
			4142	2630	677	809	26			
1	D	530	Total	C	N	O	S	0	2	0
			4147	2633	678	809	27			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
A	543	PRO	-	EXPRESSION TAG	UNP Q9P903
A	544	GLY	-	EXPRESSION TAG	UNP Q9P903
A	545	ASP	-	EXPRESSION TAG	UNP Q9P903
A	546	ASP	-	EXPRESSION TAG	UNP Q9P903
A	547	ASP	-	EXPRESSION TAG	UNP Q9P903
A	548	ASP	-	EXPRESSION TAG	UNP Q9P903
A	549	LYS	-	EXPRESSION TAG	UNP Q9P903
A	550	HIS	-	EXPRESSION TAG	UNP Q9P903
A	551	HIS	-	EXPRESSION TAG	UNP Q9P903
A	552	HIS	-	EXPRESSION TAG	UNP Q9P903
A	553	HIS	-	EXPRESSION TAG	UNP Q9P903
A	554	HIS	-	EXPRESSION TAG	UNP Q9P903
A	555	HIS	-	EXPRESSION TAG	UNP Q9P903
A	556	HIS	-	EXPRESSION TAG	UNP Q9P903
A	557	HIS	-	EXPRESSION TAG	UNP Q9P903
A	558	SER	-	EXPRESSION TAG	UNP Q9P903
A	559	GLY	-	EXPRESSION TAG	UNP Q9P903
A	560	ASP	-	EXPRESSION TAG	UNP Q9P903
B	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
B	543	PRO	-	EXPRESSION TAG	UNP Q9P903

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Chain	Residue	Modelled	Actual	Comment	Reference
B	544	GLY	-	EXPRESSION TAG	UNP Q9P903
B	545	ASP	-	EXPRESSION TAG	UNP Q9P903
B	546	ASP	-	EXPRESSION TAG	UNP Q9P903
B	547	ASP	-	EXPRESSION TAG	UNP Q9P903
B	548	ASP	-	EXPRESSION TAG	UNP Q9P903
B	549	LYS	-	EXPRESSION TAG	UNP Q9P903
B	550	HIS	-	EXPRESSION TAG	UNP Q9P903
B	551	HIS	-	EXPRESSION TAG	UNP Q9P903
B	552	HIS	-	EXPRESSION TAG	UNP Q9P903
B	553	HIS	-	EXPRESSION TAG	UNP Q9P903
B	554	HIS	-	EXPRESSION TAG	UNP Q9P903
B	555	HIS	-	EXPRESSION TAG	UNP Q9P903
B	556	HIS	-	EXPRESSION TAG	UNP Q9P903
B	557	HIS	-	EXPRESSION TAG	UNP Q9P903
B	558	SER	-	EXPRESSION TAG	UNP Q9P903
B	559	GLY	-	EXPRESSION TAG	UNP Q9P903
B	560	ASP	-	EXPRESSION TAG	UNP Q9P903
C	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
C	543	PRO	-	EXPRESSION TAG	UNP Q9P903
C	544	GLY	-	EXPRESSION TAG	UNP Q9P903
C	545	ASP	-	EXPRESSION TAG	UNP Q9P903
C	546	ASP	-	EXPRESSION TAG	UNP Q9P903
C	547	ASP	-	EXPRESSION TAG	UNP Q9P903
C	548	ASP	-	EXPRESSION TAG	UNP Q9P903
C	549	LYS	-	EXPRESSION TAG	UNP Q9P903
C	550	HIS	-	EXPRESSION TAG	UNP Q9P903
C	551	HIS	-	EXPRESSION TAG	UNP Q9P903
C	552	HIS	-	EXPRESSION TAG	UNP Q9P903
C	553	HIS	-	EXPRESSION TAG	UNP Q9P903
C	554	HIS	-	EXPRESSION TAG	UNP Q9P903
C	555	HIS	-	EXPRESSION TAG	UNP Q9P903
C	556	HIS	-	EXPRESSION TAG	UNP Q9P903
C	557	HIS	-	EXPRESSION TAG	UNP Q9P903
C	558	SER	-	EXPRESSION TAG	UNP Q9P903
C	559	GLY	-	EXPRESSION TAG	UNP Q9P903
C	560	ASP	-	EXPRESSION TAG	UNP Q9P903
D	167	KCX	LYS	MODIFIED RESIDUE	UNP Q9P903
D	543	PRO	-	EXPRESSION TAG	UNP Q9P903
D	544	GLY	-	EXPRESSION TAG	UNP Q9P903
D	545	ASP	-	EXPRESSION TAG	UNP Q9P903
D	546	ASP	-	EXPRESSION TAG	UNP Q9P903
D	547	ASP	-	EXPRESSION TAG	UNP Q9P903

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Chain	Residue	Modelled	Actual	Comment	Reference
D	548	ASP	-	EXPRESSION TAG	UNP Q9P903
D	549	LYS	-	EXPRESSION TAG	UNP Q9P903
D	550	HIS	-	EXPRESSION TAG	UNP Q9P903
D	551	HIS	-	EXPRESSION TAG	UNP Q9P903
D	552	HIS	-	EXPRESSION TAG	UNP Q9P903
D	553	HIS	-	EXPRESSION TAG	UNP Q9P903
D	554	HIS	-	EXPRESSION TAG	UNP Q9P903
D	555	HIS	-	EXPRESSION TAG	UNP Q9P903
D	556	HIS	-	EXPRESSION TAG	UNP Q9P903
D	557	HIS	-	EXPRESSION TAG	UNP Q9P903
D	558	SER	-	EXPRESSION TAG	UNP Q9P903
D	559	GLY	-	EXPRESSION TAG	UNP Q9P903
D	560	ASP	-	EXPRESSION TAG	UNP Q9P903

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

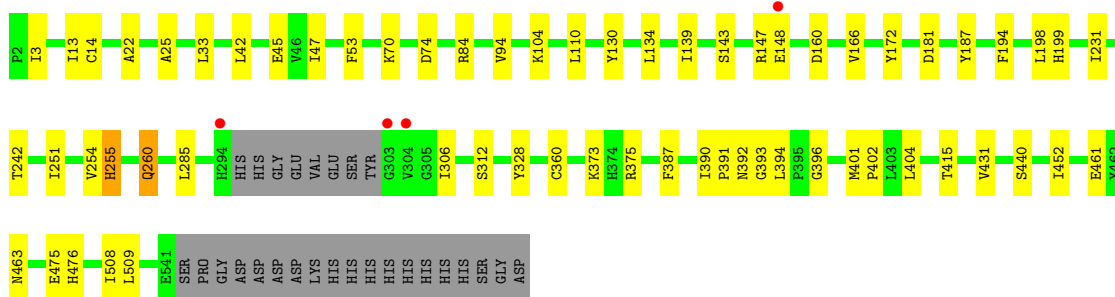
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	189	Total 189	O 189	0	0
3	B	188	Total 188	O 188	0	0
3	C	171	Total 171	O 171	0	0
3	D	133	Total 133	O 133	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

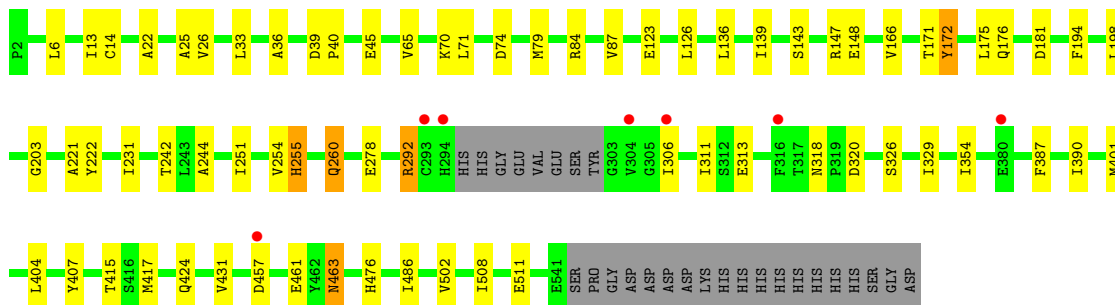
- Molecule 1: dihydropyrimidinase

Chain A: 



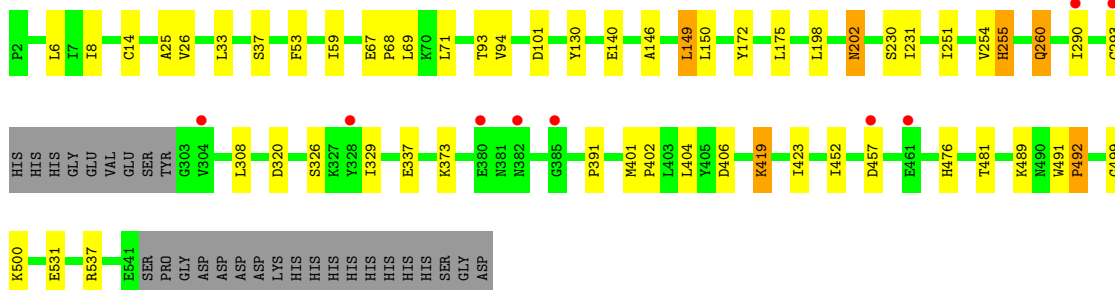
- Molecule 1: dihydropyrimidinase

Chain B: 



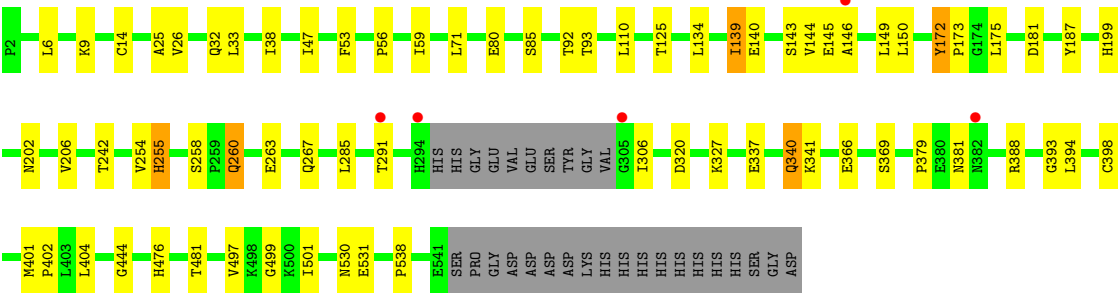
- Molecule 1: dihydropyrimidinase

Chain C: 



● Molecule 1: dihydropyrimidinase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.43Å 73.32Å 162.18Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	43.85 – 2.40 43.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.85-2.40) 99.0 (43.50-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.217 , 0.274 0.223 , 0.218	Depositor DCC
$R_{free}$ test set	4200 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.4	EDS
Estimated twinning fraction	0.126 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 83460 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	17311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.49	0/4252	0.59	0/5771
1	B	0.47	0/4260	0.60	0/5782
1	C	0.47	0/4222	0.59	0/5729
1	D	0.45	0/4234	0.57	0/5745
All	All	0.47	0/16968	0.59	0/23027

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4164	0	4093	30	0
1	B	4169	0	4104	38	0
1	C	4142	0	4072	31	0
1	D	4147	0	4077	37	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	189	0	0	2	0
3	B	188	0	0	0	0
3	C	171	0	0	3	0
3	D	133	0	0	3	0
All	All	17311	0	16346	132	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (132) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:260:GLN:HE21	1:C:260:GLN:H	1.14	0.92
1:C:140:GLU:O	1:C:146:ALA:HB2	1.78	0.83
1:D:140:GLU:O	1:D:146:ALA:HB2	1.77	0.83
1:A:198:LEU:HD12	1:A:251:ILE:HD11	1.60	0.83
1:B:198:LEU:HD12	1:B:251[A]:ILE:HD11	1.63	0.81
1:C:198:LEU:HD12	1:C:251:ILE:HD11	1.69	0.73
1:D:337:GLU:HA	1:D:340:GLN:HE22	1.54	0.73
1:A:231:ILE:HG12	1:B:242:THR:HG23	1.71	0.72
1:A:84:ARG:NH1	1:A:475:GLU:OE1	2.24	0.69
1:D:71:LEU:HD11	1:D:175:LEU:HD21	1.75	0.67
1:C:140:GLU:O	1:C:146:ALA:CB	2.43	0.66
1:B:171:THR:O	1:B:172[A]:TYR:HB2	1.97	0.64
1:B:326:SER:HA	1:B:329:ILE:HG12	1.80	0.64
1:B:70:LYS:HD2	1:B:74:ASP:OD1	1.99	0.62
1:D:140:GLU:O	1:D:146:ALA:CB	2.47	0.60
1:B:14[B]:CYS:SG	1:B:417:MET:HB3	2.44	0.57
1:A:242:THR:HG23	1:B:231:ILE:HG12	1.86	0.57
1:A:14[A]:CYS:SG	1:A:53:PHE:CD2	2.98	0.57
1:B:306:ILE:HG22	1:B:407:TYR:CZ	2.41	0.55
1:C:230:SER:HB3	1:C:260:GLN:HE22	1.71	0.55
1:A:401:MET:HB2	1:A:402:PRO:HD3	1.89	0.55
1:D:199:HIS:ND1	1:D:255:HIS:HE1	2.04	0.54
1:D:56:PRO:HG3	3:D:4642:HOH:O	2.08	0.54
1:D:149:LEU:HB2	3:D:4716:HOH:O	2.08	0.54
1:B:198:LEU:HD12	1:B:251[A]:ILE:CD1	2.35	0.53
1:C:149:LEU:HB3	3:C:3734:HOH:O	2.08	0.53
1:B:25:ALA:HB3	1:B:33:LEU:HB3	1.91	0.53
1:D:145:GLU:HA	1:D:145:GLU:OE1	2.07	0.53
1:B:313:GLU:HA	1:B:318:ASN:ND2	2.24	0.52
1:C:59:ILE:HG12	1:C:93:THR:HB	1.91	0.52
1:D:110:LEU:HB3	1:D:134:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:254:VAL:HG23	1:B:255:HIS:CE1	2.45	0.52
1:B:260:GLN:H	1:B:260:GLN:NE2	2.08	0.51
1:D:143:SER:C	1:D:145:GLU:H	2.13	0.51
1:C:260:GLN:HE21	1:C:260:GLN:N	1.96	0.51
1:B:13:ILE:HD12	1:B:22:ALA:HB3	1.94	0.49
1:A:387:PHE:HA	1:A:390:ILE:HD12	1.94	0.49
1:A:440:SER:HB3	3:C:3658:HOH:O	2.10	0.49
1:C:406:ASP:OD1	1:C:489:LYS:NZ	2.34	0.49
1:D:146:ALA:O	1:D:150:LEU:HB2	2.12	0.49
1:C:231:ILE:HG12	1:D:242:THR:HG23	1.93	0.49
1:C:401:MET:HB2	1:C:402:PRO:HD3	1.95	0.48
1:C:6:LEU:HB3	1:C:26:VAL:HB	1.96	0.48
1:A:147:ARG:HD2	1:A:187:TYR:CE2	2.48	0.48
1:C:71:LEU:HD11	1:C:175:LEU:HD21	1.94	0.48
1:D:327:LYS:O	1:D:394:LEU:HD22	2.14	0.48
1:B:401:MET:HA	1:B:424:GLN:HE22	1.79	0.47
1:B:39:ASP:OD2	1:B:40:PRO:HD2	2.14	0.47
1:C:260:GLN:NE2	1:C:260:GLN:H	1.95	0.47
1:D:47:ILE:HD11	1:D:501:ILE:HD11	1.96	0.47
1:C:290:ILE:HD13	1:C:308:LEU:HD22	1.96	0.47
1:C:419:LYS:O	1:C:423:ILE:HG12	2.14	0.47
1:D:139:ILE:HG13	1:D:181:ASP:HB3	1.95	0.47
1:D:9:LYS:NZ	1:D:38:ILE:O	2.46	0.47
1:B:387:PHE:HA	1:B:390:ILE:HD12	1.96	0.47
1:D:80:GLU:HG3	1:D:125:THR:O	2.14	0.47
1:D:14[A]:CYS:SG	1:D:53:PHE:CD2	3.08	0.47
1:B:84:ARG:NH1	1:B:508:ILE:HG21	2.30	0.47
1:D:401:MET:HB2	1:D:402:PRO:HD3	1.97	0.47
1:D:59:ILE:HG12	1:D:93:THR:HB	1.96	0.46
1:B:87:VAL:HG11	1:B:502:VAL:HG12	1.98	0.46
1:D:187:TYR:CE1	1:D:538:PRO:HB3	2.50	0.46
1:C:69:LEU:HD11	1:C:101:ASP:HB2	1.98	0.46
1:A:199:HIS:ND1	1:A:255:HIS:HE1	2.13	0.46
1:C:537:ARG:HB2	3:C:3708:HOH:O	2.16	0.46
1:C:202:ASN:C	1:C:202:ASN:HD22	2.20	0.45
1:A:166:VAL:HG23	1:A:194:PHE:HD2	1.81	0.45
1:A:260:GLN:NE2	1:A:260:GLN:H	2.14	0.45
1:B:244:ALA:HB2	1:B:251[B]:ILE:HG13	1.97	0.45
1:B:306:ILE:HD11	1:B:311:ILE:HD11	1.99	0.45
1:A:387:PHE:HA	1:A:390:ILE:CD1	2.47	0.44
1:D:393:GLY:O	1:D:394:LEU:HD23	2.16	0.44
1:B:166:VAL:HG23	1:B:194:PHE:HD1	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:530:ASN:ND2	3:D:4671:HOH:O	2.50	0.44
1:C:8:ILE:HD13	1:C:452:ILE:HD11	2.00	0.44
1:B:260:GLN:H	1:B:260:GLN:HE21	1.64	0.44
1:A:139:ILE:HG13	1:A:181:ASP:HB3	2.00	0.44
1:B:6:LEU:HB3	1:B:26:VAL:HB	1.99	0.44
1:A:74:ASP:O	1:A:375:ARG:NH2	2.51	0.44
1:B:401:MET:HA	1:B:424:GLN:NE2	2.33	0.44
1:D:202:ASN:O	1:D:206:VAL:HG23	2.18	0.44
1:A:508:ILE:HG22	3:A:1661:HOH:O	2.16	0.44
1:A:509:LEU:HD23	3:A:1790:HOH:O	2.17	0.44
1:B:221:ALA:HB1	1:B:329:ILE:HD11	2.00	0.44
1:B:136:LEU:HD22	1:B:166:VAL:HG11	2.00	0.44
1:A:110:LEU:HB3	1:A:134:LEU:HD21	2.00	0.44
1:B:79:MET:HG3	1:B:126:LEU:HD22	1.99	0.43
1:D:85:SER:OG	1:D:398:CYS:HB2	2.18	0.43
1:C:25:ALA:HB3	1:C:33:LEU:HB3	2.00	0.43
1:C:230:SER:HB3	1:C:260:GLN:NE2	2.33	0.43
1:B:306:ILE:HD12	1:B:486:ILE:HG21	2.01	0.43
1:C:491:TRP:CG	1:C:492:PRO:HD2	2.54	0.43
1:B:71:LEU:HD11	1:B:175:LEU:HD21	2.00	0.43
1:C:254:VAL:HG23	1:C:255:HIS:CE1	2.53	0.43
1:B:143:SER:O	1:B:147:ARG:CG	2.66	0.43
1:B:139:ILE:HG13	1:B:181:ASP:HB3	2.00	0.43
1:C:14:CYS:SG	1:C:53:PHE:CD2	3.12	0.43
1:C:94:VAL:O	1:C:130:TYR:HA	2.19	0.43
1:A:147:ARG:HD2	1:A:187:TYR:CD2	2.54	0.43
1:B:387:PHE:HA	1:B:390:ILE:CD1	2.49	0.43
1:B:463:ASN:N	1:B:463:ASN:OD1	2.52	0.43
1:A:328:TYR:HA	1:A:394:LEU:HD21	2.00	0.43
1:D:258:SER:OG	1:D:260:GLN:HG2	2.19	0.42
1:C:146:ALA:O	1:C:150:LEU:HB2	2.19	0.42
1:D:379:PRO:C	1:D:381:ASN:H	2.22	0.42
1:A:3:ILE:HG22	1:A:42:LEU:O	2.19	0.42
1:D:6:LEU:HB3	1:D:26:VAL:HB	2.02	0.42
1:A:285:LEU:HB3	1:A:306:ILE:HD12	2.00	0.42
1:D:285:LEU:HD22	1:D:306:ILE:HG13	2.01	0.42
1:B:222:TYR:CD1	1:B:292:ARG:HG2	2.55	0.41
1:D:92:THR:HG22	1:D:497:VAL:HG22	2.02	0.41
1:B:36:ALA:HB2	1:D:444:GLY:HA3	2.01	0.41
1:A:143:SER:O	1:A:147:ARG:HG3	2.19	0.41
1:A:94:VAL:O	1:A:130:TYR:HA	2.20	0.41
1:A:360:CYS:HB3	1:A:393:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:176:GLN:OE1	1:B:203:GLY:HA3	2.19	0.41
1:D:26:VAL:HG11	1:D:499:GLY:HA2	2.01	0.41
1:A:47:ILE:HG21	1:A:452:ILE:HD13	2.02	0.41
1:D:254:VAL:HG23	1:D:255:HIS:CE1	2.56	0.41
1:C:67:GLU:HB2	1:C:68:PRO:HD2	2.01	0.41
1:A:373:LYS:HD3	1:A:391:PRO:HG2	2.03	0.41
1:D:172:TYR:HA	1:D:173:PRO:HD3	1.95	0.41
1:A:25:ALA:HB3	1:A:33:LEU:HB3	2.02	0.41
1:D:25:ALA:HB3	1:D:33:LEU:HB3	2.02	0.41
1:C:26:VAL:HG11	1:C:499:GLY:HA2	2.02	0.41
1:A:13:ILE:HD12	1:A:22:ALA:HB3	2.02	0.41
1:B:278:GLU:HG3	1:B:354:ILE:HG13	2.02	0.41
1:C:373:LYS:HA	1:C:391:PRO:HG2	2.03	0.40
1:D:285:LEU:HB3	1:D:306:ILE:HD12	2.03	0.40
1:D:263:GLU:O	1:D:267:GLN:HG3	2.22	0.40
1:A:254:VAL:HG23	1:A:255:HIS:CE1	2.56	0.40
1:C:326:SER:HA	1:C:329:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

## 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	529/559 (95%)	510 (96%)	15 (3%)	4 (1%)	27	39
1	B	530/559 (95%)	512 (97%)	16 (3%)	2 (0%)	43	61
1	C	526/559 (94%)	506 (96%)	18 (3%)	2 (0%)	43	61
1	D	527/559 (94%)	505 (96%)	19 (4%)	3 (1%)	33	47
All	All	2112/2236 (94%)	2033 (96%)	68 (3%)	11 (0%)	43	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	144	VAL

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Mol	Chain	Res	Type
1	A	172[A]	TYR
1	A	172[B]	TYR
1	A	255	HIS
1	B	172[A]	TYR
1	B	172[B]	TYR
1	C	172	TYR
1	D	172	TYR
1	D	255	HIS
1	C	255	HIS
1	A	396	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	457/479 (95%)	443 (97%)	14 (3%)	52	74
1	B	458/479 (96%)	442 (96%)	16 (4%)	48	69
1	C	454/479 (95%)	439 (97%)	15 (3%)	50	71
1	D	456/479 (95%)	442 (97%)	14 (3%)	52	74
All	All	1825/1916 (95%)	1766 (97%)	59 (3%)	51	72

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	70	LYS
1	A	104	LYS
1	A	148	GLU
1	A	160	ASP
1	A	260	GLN
1	A	312	SER
1	A	392	ASN
1	A	404	LEU
1	A	415	THR
1	A	431	VAL
1	A	461	GLU

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Mol	Chain	Res	Type
1	A	463	ASN
1	A	476	HIS
1	B	45	GLU
1	B	65	VAL
1	B	123	GLU
1	B	148	GLU
1	B	255	HIS
1	B	260	GLN
1	B	292	ARG
1	B	320	ASP
1	B	404	LEU
1	B	415	THR
1	B	431	VAL
1	B	457	ASP
1	B	461	GLU
1	B	463	ASN
1	B	476	HIS
1	B	511	GLU
1	C	37	SER
1	C	149	LEU
1	C	202	ASN
1	C	260	GLN
1	C	293	CYS
1	C	320	ASP
1	C	337	GLU
1	C	404	LEU
1	C	419	LYS
1	C	457	ASP
1	C	476	HIS
1	C	481	THR
1	C	492	PRO
1	C	500	LYS
1	C	531	GLU
1	D	32	GLN
1	D	139	ILE
1	D	260	GLN
1	D	291	THR
1	D	320	ASP
1	D	340	GLN
1	D	341	LYS
1	D	366	GLU
1	D	369	SER

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Mol	Chain	Res	Type
1	D	388	ARG
1	D	404	LEU
1	D	476	HIS
1	D	481	THR
1	D	531	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	267	GLN
1	A	294	HIS
1	A	318	ASN
1	B	260	GLN
1	B	318	ASN
1	B	424	GLN
1	C	27	ASN
1	C	202	ASN
1	C	260	GLN
1	D	267	GLN
1	D	340	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	167	1,2	11,11,12	5.79	2 (18%)	10,12,14	1.64	3 (30%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	B	167	1,2	11,11,12	5.21	2 (18%)	10,12,14	1.88	3 (30%)
1	KCX	C	167	1,2	11,11,12	5.38	2 (18%)	10,12,14	1.70	3 (30%)
1	KCX	D	167	1,2	11,11,12	5.03	2 (18%)	10,12,14	1.75	2 (20%)

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	167	1,2	-	0/8/10/12	0/0/0/0
1	KCX	B	167	1,2	-	0/8/10/12	0/0/0/0
1	KCX	C	167	1,2	-	0/8/10/12	0/0/0/0
1	KCX	D	167	1,2	-	0/8/10/12	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	KCX	O-C	18.86	1.24	1.11
1	C	167	KCX	O-C	17.50	1.23	1.11
1	B	167	KCX	O-C	16.90	1.23	1.11
1	D	167	KCX	O-C	16.30	1.22	1.11
1	B	167	KCX	CA-C	2.54	1.53	1.48
1	A	167	KCX	CA-C	2.53	1.53	1.48
1	C	167	KCX	CA-C	2.46	1.52	1.48
1	D	167	KCX	CA-C	2.07	1.52	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	KCX	OQ1-CX-NZ	-3.58	118.99	124.94
1	C	167	KCX	OQ2-CX-NZ	3.49	120.67	116.33
1	D	167	KCX	OQ2-CX-NZ	3.48	120.67	116.33
1	B	167	KCX	OQ1-CX-NZ	-3.33	119.40	124.94
1	B	167	KCX	OQ2-CX-NZ	3.24	120.36	116.33
1	A	167	KCX	OQ1-CX-NZ	-2.94	120.04	124.94
1	A	167	KCX	C-CA-N	-2.82	111.02	113.83
1	C	167	KCX	OQ2-CX-OQ1	-2.72	118.77	122.17
1	C	167	KCX	OQ1-CX-NZ	-2.63	120.56	124.94
1	A	167	KCX	OQ2-CX-NZ	2.56	119.52	116.33
1	B	167	KCX	C-CA-N	-2.48	111.35	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	532/559 (95%)	0.02	4 (0%) 83 82	31, 36, 38, 45	0
1	B	532/559 (95%)	0.02	7 (1%) 74 73	31, 36, 38, 42	0
1	C	531/559 (94%)	0.09	9 (1%) 67 65	31, 36, 38, 42	0
1	D	530/559 (94%)	0.07	5 (0%) 81 81	31, 36, 38, 42	0
All	All	2125/2236 (95%)	0.05	25 (1%) 75 75	31, 36, 38, 45	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	ALA	6.6
1	C	304	VAL	3.9
1	B	294	HIS	3.9
1	B	306	ILE	3.4
1	C	457	ASP	3.2
1	B	293	CYS	3.2
1	A	294	HIS	3.1
1	A	303	GLY	3.0
1	D	382	ASN	2.9
1	D	294	HIS	2.7
1	B	457	ASP	2.6
1	D	291	THR	2.6
1	A	304	VAL	2.5
1	C	293	CYS	2.5
1	C	382	ASN	2.4
1	C	328	TYR	2.4
1	C	461	GLU	2.4
1	B	380	GLU	2.3
1	C	385	GLY	2.3
1	A	148	GLU	2.3
1	D	305	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	316	PHE	2.1
1	C	380	GLU	2.1
1	B	304	VAL	2.1
1	C	290	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	C	167	12/13	0.18	0.62	35,36,44,44	3
1	KCX	D	167	12/13	0.17	0.20	35,36,44,44	3
1	KCX	A	167	12/13	0.15	0.01	35,36,44,45	3
1	KCX	B	167	12/13	0.13	-0.76	35,35,44,44	3

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	D	602	1/1	0.14	-0.49	46,46,46,46	1
2	ZN	B	602	1/1	0.11	-1.23	46,46,46,46	1
2	ZN	C	602	1/1	0.08	-2.16	45,45,45,45	1
2	ZN	D	601	1/1	0.04	-2.60	44,44,44,44	1
2	ZN	A	602	1/1	0.08	-2.68	45,45,45,45	1
2	ZN	C	601	1/1	0.04	-3.97	44,44,44,44	1
2	ZN	A	601	1/1	0.03	-4.05	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	B	601	1/1	0.03	-4.21	43,43,43,43	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.