



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:12 PM GMT

PDB ID : 1J79  
Title : Molecular Structure of Dihydroorotase: A Paradigm for Catalysis Through the Use of a Binuclear Metal Center  
Authors : Thoden, J.B.; Phillips Jr., G.N.; Neal, T.M.; Raushel, F.M.; Holden, H.M.  
Deposited on : 2001-05-16  
Resolution : 1.70 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

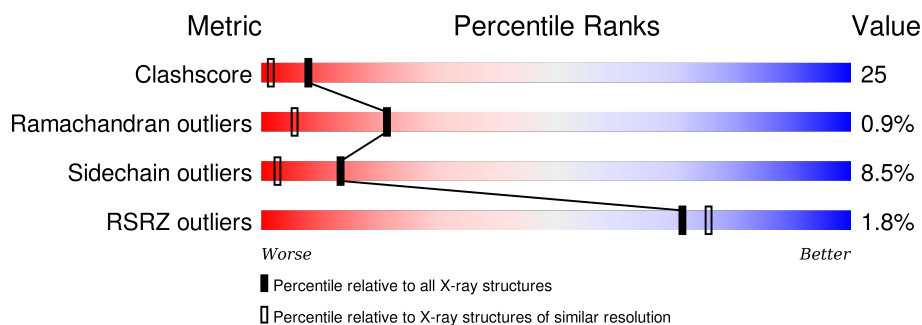
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	347	
1	B	347	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NCD	A	950	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6212 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 dihydroorotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	11	0
			2751	1742	491	502	16			
1	B	339	Total	C	N	O	S	0	3	0
			2691	1703	479	493	16			

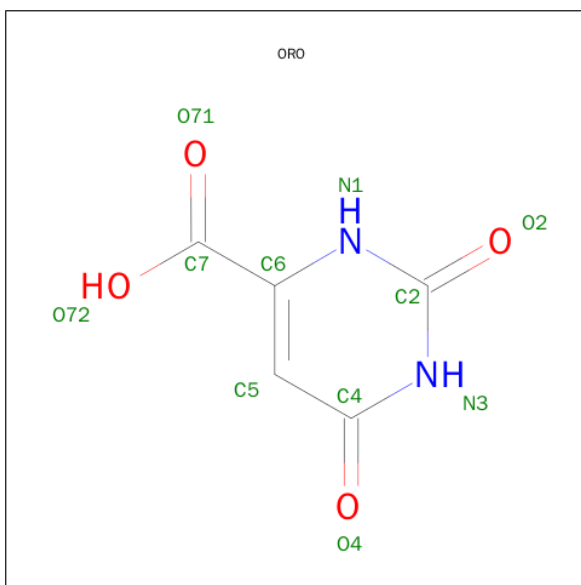
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	PRO	GLY	SEE REMARK 999	UNP P05020
A	102	KCX	LYS	MODIFIED RESIDUE	UNP P05020
A	119	VAL	ILE	SEE REMARK 999	UNP P05020
A	243	GLN	ASN	SEE REMARK 999	UNP P05020
B	69	PRO	GLY	SEE REMARK 999	UNP P05020
B	102	KCX	LYS	MODIFIED RESIDUE	UNP P05020
B	119	VAL	ILE	SEE REMARK 999	UNP P05020
B	243	GLN	ASN	SEE REMARK 999	UNP P05020

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

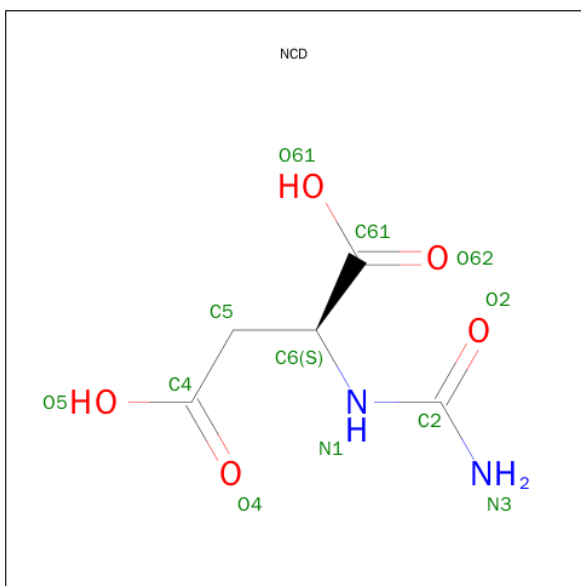
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is OROTIC ACID (three-letter code: ORO) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is N-CARBAMOYL-L-ASPARTATE (three-letter code: NCD) (formula:  $C_5H_8N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			12	5	2	5		
4	A	1	Total	C	N	O	0	0
			12	5	2	5		

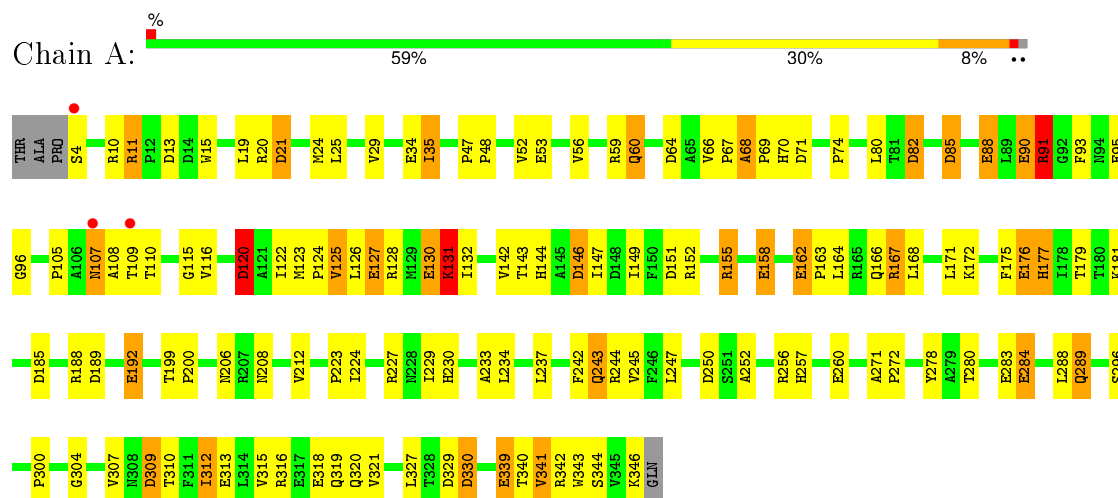
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	413	Total 413	O 413	0	0
5	B	318	Total 318	O 318	0	0

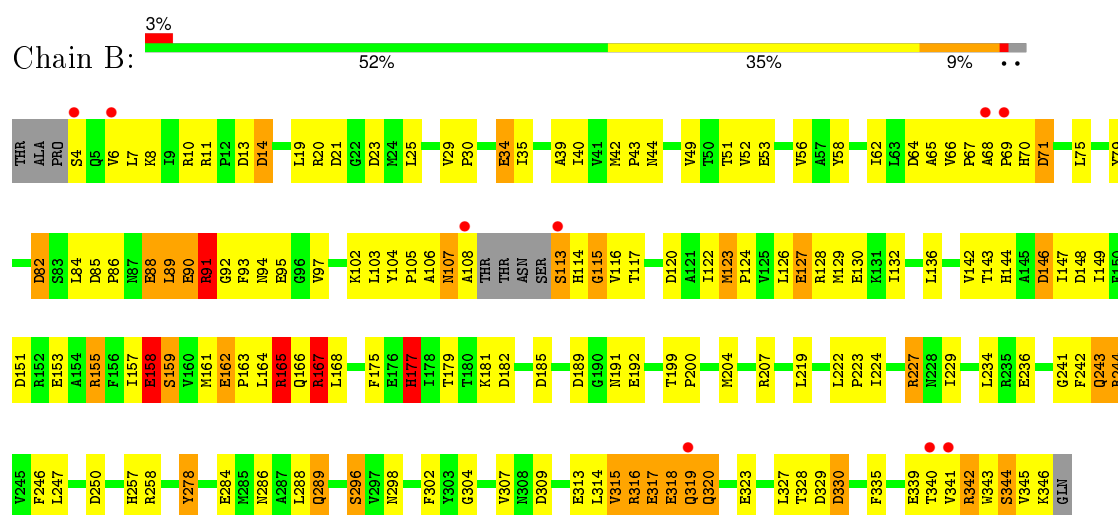
### 3 Residue-property plots

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: dihydroorotase



- Molecule 1: dihydroorotase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.60 Å 78.80 Å 180.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 29.58 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.70) 95.8 (29.58-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.80 (at 1.50 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.191 , 0.258 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 110.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 113580 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ORO, ZN, NCD, 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	0.92	14/2845 (0.5%)	1.31	38/3869 (1.0%)
1	B	0.93	14/2752 (0.5%)	1.33	46/3740 (1.2%)
All	All	0.93	28/5597 (0.5%)	1.32	84/7609 (1.1%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	GLU	CD-OE2	7.46	1.33	1.25
1	A	260	GLU	CD-OE2	6.88	1.33	1.25
1	A	158	GLU	CD-OE2	6.83	1.33	1.25
1	B	153	GLU	CD-OE2	6.65	1.32	1.25
1	B	158	GLU	CD-OE2	6.60	1.32	1.25
1	A	130	GLU	CD-OE2	6.40	1.32	1.25
1	B	127	GLU	CD-OE2	6.20	1.32	1.25
1	A	192	GLU	CD-OE2	6.19	1.32	1.25
1	A	284	GLU	CD-OE2	6.13	1.32	1.25
1	A	339	GLU	CD-OE2	5.75	1.31	1.25
1	B	317	GLU	CD-OE2	5.74	1.31	1.25
1	B	162	GLU	CD-OE2	5.73	1.31	1.25
1	B	236	GLU	CD-OE2	5.69	1.31	1.25
1	A	53	GLU	CD-OE2	5.68	1.31	1.25
1	B	53	GLU	CD-OE2	5.68	1.31	1.25
1	A	318	GLU	CD-OE2	5.65	1.31	1.25
1	A	88	GLU	CD-OE2	5.62	1.31	1.25
1	B	34	GLU	CD-OE2	5.60	1.31	1.25
1	A	313	GLU	CD-OE2	5.55	1.31	1.25
1	B	318	GLU	CD-OE2	5.51	1.31	1.25
1	B	323	GLU	CD-OE2	5.51	1.31	1.25
1	B	192	GLU	CD-OE2	5.45	1.31	1.25
1	A	127	GLU	CD-OE2	5.44	1.31	1.25
1	B	130	GLU	CD-OE2	5.41	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	GLU	CD-OE2	5.11	1.31	1.25
1	B	90	GLU	CD-OE2	5.10	1.31	1.25
1	A	34	GLU	CD-OE2	5.08	1.31	1.25
1	B	284	GLU	CD-OE2	5.02	1.31	1.25

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	256[A]	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	A	256[B]	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	B	71	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	167	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	309	ASP	CB-CG-OD1	8.04	125.53	118.30
1	B	71	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	A	20	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	146	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	A	82	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	330	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	330	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	151	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	309	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	21	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	B	82	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	82	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	148	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	166	GLN	CB-CA-C	6.88	124.16	110.40
1	A	189	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	256[A]	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	256[B]	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	185	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	14	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	329	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	B	14	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	20	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	165	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	151	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	329	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	A	13	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	278	TYR	CB-CG-CD1	-6.39	117.16	121.00
1	A	120	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	82	ASP	CB-CG-OD1	6.34	124.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	146	ASP	N-CA-CB	6.28	121.90	110.60
1	B	13	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	B	258	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	189	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	151	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	227	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	309	ASP	CB-CG-OD1	6.08	123.78	118.30
1	A	309	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	185	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	64	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	120	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	252	ALA	N-CA-CB	-5.72	102.09	110.10
1	B	23	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	207	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	107[A]	ASN	N-CA-CB	5.67	120.80	110.60
1	A	107[B]	ASN	N-CA-CB	5.67	120.80	110.60
1	B	64	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	64	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	329	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	330	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	B	278	TYR	CB-CG-CD2	5.61	124.37	121.00
1	B	330	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	182	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	B	151	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	21	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	131[A]	LYS	CB-CA-C	5.49	121.38	110.40
1	A	131[B]	LYS	CB-CA-C	5.49	121.38	110.40
1	A	91	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	20	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	250	ASP	N-CA-CB	5.43	120.38	110.60
1	A	146	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	296	SER	N-CA-CB	-5.38	102.43	110.50
1	A	250	ASP	N-CA-CB	5.36	120.25	110.60
1	A	250	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	120	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	146	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	64	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	185	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	120	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	85	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	244	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	155[A]	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	155[B]	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	250	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	342	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	207	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	189	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	316	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	2751	0	2725	121	0
1	B	2691	0	2658	146	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	3	0	0
4	A	12	0	6	5	0
4	B	12	0	6	2	0
5	A	413	0	0	12	1
5	B	318	0	0	19	0
All	All	6212	0	5398	270	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 25.

All (270) 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:243:GLN:NE2	1:B:243:GLN:H	1.50	1.10
1:B:29:VAL:HG23	1:B:30:PRO:HD3	1.33	1.04
1:B:6:VAL:HG12	1:B:315:VAL:HG13	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLN:HG2	1:B:320:GLN:H	1.38	0.88
1:B:123:MET:HE3	1:B:167:ARG:HD2	1.55	0.88
1:B:123:MET:HE3	1:B:167:ARG:CD	2.03	0.87
1:B:93:PHE:CD2	1:B:132:ILE:HD12	2.10	0.86
1:B:243:GLN:HE21	1:B:243:GLN:H	1.19	0.85
1:B:52:VAL:HG13	1:B:97:VAL:HG21	1.60	0.84
1:A:289:GLN:HE21	1:A:289:GLN:H	1.21	0.84
1:B:68:ALA:HB3	1:B:69:PRO:HD3	1.57	0.84
1:A:212:VAL:HG11	4:A:950:NCD:O62	1.75	0.84
1:A:142[B]:VAL:HG23	1:A:147:ILE:HD13	1.62	0.81
1:B:6:VAL:HG12	1:B:315:VAL:CG1	2.11	0.80
1:B:7:LEU:HD11	1:B:288:LEU:HD22	1.65	0.79
1:A:142[B]:VAL:CG2	1:A:147:ILE:HD13	2.14	0.78
1:A:91:ARG:O	1:A:95:GLU:HG3	1.84	0.77
1:B:35:ILE:HD11	1:B:345:VAL:HG11	1.64	0.77
1:B:25:LEU:O	1:B:29:VAL:HG22	1.85	0.77
1:A:11[A]:ARG:HD2	1:A:310:THR:OG1	1.85	0.76
1:A:316:ARG:HB2	1:A:343:TRP:CZ3	2.21	0.75
1:B:29:VAL:CG2	1:B:30:PRO:HD3	2.14	0.75
1:B:52:VAL:CG1	1:B:97:VAL:HG21	2.15	0.75
1:B:243:GLN:N	1:B:243:GLN:HE21	1.85	0.75
1:B:103:LEU:CD1	1:B:116:VAL:HG21	2.17	0.74
1:A:127:GLU:O	1:A:131[A]:LYS:HD3	1.87	0.74
1:A:107[A]:ASN:OD1	1:A:109:THR:HB	1.87	0.73
1:B:316:ARG:NH2	1:B:342:ARG:HD3	2.04	0.73
1:B:84:LEU:HD12	5:B:1185:HOH:O	1.87	0.73
1:A:309:ASP:HA	5:A:1213:HOH:O	1.90	0.71
1:A:155[B]:ARG:HG2	5:A:1400:HOH:O	1.90	0.71
1:A:96:GLY:C	5:A:1299:HOH:O	2.28	0.71
1:A:25[B]:LEU:HD12	1:A:29:VAL:HG23	1.72	0.71
1:B:319:GLN:HG2	1:B:320:GLN:N	2.07	0.70
4:B:411:NCD:C4	4:B:411:NCD:H31	2.04	0.70
1:B:243:GLN:N	1:B:243:GLN:NE2	2.34	0.70
1:B:52:VAL:HG22	1:B:92:GLY:HA3	1.73	0.70
1:B:108:ALA:C	1:B:113:SER:HA	2.11	0.70
1:B:49:VAL:HG22	5:B:1551:HOH:O	1.92	0.69
1:B:122:ILE:HD12	1:B:126:LEU:HD21	1.74	0.69
1:A:208:ASN:HB3	4:A:950:NCD:H61	1.73	0.69
1:A:91:ARG:HD2	1:A:95:GLU:OE2	1.93	0.69
1:A:316:ARG:HB2	1:A:343:TRP:CH2	2.28	0.68
1:A:11[A]:ARG:HE	1:A:312:ILE:HD12	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PRO:O	1:B:204:MET:HG3	1.94	0.67
1:A:128:ARG:O	1:A:132:ILE:HG12	1.93	0.67
1:B:35:ILE:CD1	1:B:345:VAL:HG11	2.25	0.66
1:B:106:ALA:C	1:B:107:ASN:HD22	1.99	0.66
1:B:103:LEU:HD11	1:B:116:VAL:HG21	1.77	0.65
1:B:105:PRO:O	1:B:107:ASN:ND2	2.30	0.65
1:B:114:HIS:ND1	5:B:1426:HOH:O	2.29	0.64
1:B:123:MET:HE3	1:B:167:ARG:NE	2.13	0.64
1:B:85:ASP:O	1:B:88:GLU:HB2	1.97	0.63
1:A:242:PHE:HD2	1:A:245[B]:VAL:HG13	1.62	0.63
1:B:91[B]:ARG:HD2	1:B:95:GLU:OE2	1.99	0.62
1:A:188:ARG:NH2	5:A:1519:HOH:O	2.31	0.62
1:A:68:ALA:HB3	1:A:69:PRO:HD3	1.81	0.62
1:A:131[B]:LYS:HD2	5:A:1605:HOH:O	1.98	0.61
1:A:144:HIS:HB2	1:A:147:ILE:HD12	1.83	0.61
1:B:62:ILE:O	1:B:66:VAL:HG23	2.01	0.61
1:A:242:PHE:CD2	1:A:245[B]:VAL:HG13	2.36	0.61
1:A:123:MET:HA	1:A:123:MET:HE3	1.83	0.61
1:A:280:THR:O	1:A:284:GLU:HG3	2.00	0.60
1:A:11[A]:ARG:NE	1:A:312:ILE:HD12	2.16	0.60
1:A:107[B]:ASN:ND2	1:A:110:THR:OG1	2.29	0.59
1:B:162:GLU:HB3	1:B:163:PRO:HD3	1.84	0.59
1:B:313:GLU:OE2	1:B:346:LYS:HE3	2.02	0.59
1:A:24:MET:HE2	5:A:1697:HOH:O	2.02	0.59
1:A:315:VAL:HG23	1:A:346:LYS:HB2	1.85	0.59
1:A:164:LEU:CD1	1:A:168:LEU:HD12	2.32	0.59
1:B:25:LEU:HD12	1:B:29:VAL:HG13	1.83	0.58
1:A:90:GLU:OE1	1:A:128:ARG:HD2	2.04	0.58
1:B:142:VAL:CG2	1:B:147:ILE:HD13	2.33	0.58
1:B:302:PHE:HB2	5:B:1323:HOH:O	2.02	0.58
1:B:315:VAL:CG2	1:B:346:LYS:HB3	2.34	0.57
1:A:283:GLU:OE1	1:A:342:ARG:NH1	2.29	0.57
1:B:177:HIS:CE1	1:B:223:PRO:HD3	2.41	0.56
1:B:90:GLU:O	1:B:94:ASN:N	2.35	0.56
1:A:164:LEU:HD11	1:A:168:LEU:HD12	1.88	0.56
1:A:125:VAL:HG12	1:A:126:LEU:N	2.20	0.56
1:B:43:PRO:HB2	1:B:79:TYR:HB2	1.88	0.56
1:B:8:LYS:HG3	1:B:313:GLU:HG3	1.88	0.55
1:B:29:VAL:HG23	1:B:30:PRO:CD	2.22	0.55
1:A:181:LYS:HB2	1:A:233:ALA:CB	2.36	0.55
1:B:144:HIS:N	1:B:147:ILE:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:N	1:B:314:LEU:O	2.34	0.54
1:A:107[B]:ASN:HB2	1:A:110:THR:OG1	2.07	0.54
1:B:144:HIS:HB3	1:B:147:ILE:CD1	2.36	0.54
1:B:161:MET:O	1:B:164:LEU:HB3	2.08	0.54
1:A:319:GLN:O	1:A:341:VAL:N	2.30	0.54
1:B:315:VAL:HG21	1:B:346:LYS:HB3	1.90	0.54
1:B:40:ILE:HD13	1:B:75:LEU:HB2	1.90	0.53
1:A:162:GLU:N	1:A:163:PRO:HD2	2.23	0.53
1:B:90:GLU:O	1:B:93:PHE:HB3	2.09	0.53
1:A:237:LEU:HD21	1:A:245[B]:VAL:HG11	1.89	0.53
1:A:144:HIS:HB2	1:A:147:ILE:CD1	2.39	0.53
1:A:142[B]:VAL:HG21	1:A:147:ILE:HD13	1.91	0.53
1:A:316:ARG:HH21	1:A:342:ARG:HD3	1.72	0.53
1:B:241:GLY:O	1:B:242:PHE:C	2.47	0.53
1:B:107:ASN:HD22	1:B:107:ASN:N	2.05	0.53
1:A:164:LEU:HD11	1:A:168:LEU:CD1	2.39	0.53
1:B:335:PHE:HD1	5:B:1320:HOH:O	1.92	0.53
1:A:25[B]:LEU:CD1	1:A:29:VAL:HG23	2.38	0.53
1:B:167:ARG:HG2	1:B:167:ARG:O	2.08	0.53
1:B:52:VAL:HG22	1:B:92:GLY:CA	2.38	0.53
1:A:11[B]:ARG:NH1	1:A:71:ASP:O	2.42	0.52
1:B:242:PHE:CZ	1:B:244:ARG:HB2	2.44	0.52
1:B:107:ASN:ND2	1:B:143:THR:HG21	2.24	0.52
1:B:165:ARG:NH2	5:B:1448:HOH:O	2.25	0.52
1:B:95:GLU:HB2	1:B:97:VAL:HG23	1.91	0.52
1:B:162:GLU:O	1:B:163:PRO:C	2.48	0.52
1:B:243:GLN:CD	1:B:243:GLN:H	2.12	0.51
1:A:237:LEU:CD2	1:A:245[B]:VAL:HG11	2.40	0.51
1:B:222:LEU:HA	1:B:223:PRO:C	2.30	0.51
1:B:90:GLU:HG2	1:B:94:ASN:ND2	2.25	0.51
1:A:181:LYS:HB2	1:A:233:ALA:HB2	1.93	0.51
1:A:123:MET:CE	1:A:123:MET:HA	2.41	0.51
1:B:85:ASP:OD2	1:B:86:PRO:HD2	2.10	0.51
1:B:67:PRO:HG2	1:B:70:HIS:CE1	2.45	0.51
1:A:11[A]:ARG:HG3	1:A:312:ILE:HD13	1.93	0.50
1:A:316:ARG:HG2	1:A:316:ARG:O	2.11	0.50
1:A:128:ARG:O	1:A:128:ARG:HG3	2.11	0.50
1:A:47:PRO:HB2	1:A:48:PRO:HD2	1.92	0.50
1:A:179:THR:HA	1:A:234:LEU:HD11	1.93	0.50
1:A:52:VAL:O	1:A:56:VAL:HG23	2.12	0.49
1:A:212:VAL:HG22	1:B:149:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASP:HA	1:A:25[A]:LEU:HB2	1.94	0.49
1:B:162:GLU:HB3	1:B:163:PRO:CD	2.43	0.49
1:A:283:GLU:OE2	1:A:316:ARG:NH1	2.46	0.49
1:B:123:MET:N	1:B:124:PRO:HD2	2.28	0.49
1:A:289:GLN:HE21	1:A:289:GLN:N	2.01	0.49
1:B:58:TYR:O	1:B:62:ILE:HG13	2.13	0.49
1:B:144:HIS:H	1:B:147:ILE:HD12	1.78	0.49
1:B:162:GLU:OE2	1:B:166:GLN:NE2	2.45	0.49
1:B:25:LEU:CD1	1:B:29:VAL:HG13	2.43	0.48
1:B:6:VAL:HA	1:B:314:LEU:O	2.13	0.48
1:B:92:GLY:O	1:B:97:VAL:N	2.42	0.48
1:B:179:THR:CG2	1:B:223:PRO:HG2	2.44	0.48
1:A:70:HIS:CD2	1:A:70:HIS:N	2.80	0.48
1:A:35:ILE:HD13	5:A:1494:HOH:O	2.12	0.48
1:A:131[A]:LYS:HE3	5:A:1605:HOH:O	2.12	0.48
1:A:199:THR:HB	1:A:200:PRO:HD2	1.96	0.48
1:A:120:ASP:CG	1:A:167:ARG:HH22	2.16	0.48
1:A:320:GLN:HA	1:A:339:GLU:O	2.14	0.48
1:B:71:ASP:OD2	5:B:1557:HOH:O	2.20	0.47
4:A:950:NCD:O5	4:A:950:NCD:O61	2.32	0.47
1:B:142:VAL:HG21	1:B:147:ILE:HD13	1.95	0.47
1:B:304:GLY:HA2	5:B:1657:HOH:O	2.15	0.47
1:B:179:THR:HG23	1:B:223:PRO:HG2	1.97	0.47
1:B:90:GLU:HG2	1:B:94:ASN:HD21	1.80	0.47
1:B:88:GLU:HA	1:B:88:GLU:OE1	2.13	0.47
1:B:124:PRO:HG2	5:B:1439:HOH:O	2.15	0.47
1:A:247:LEU:HG	1:A:278:TYR:CE1	2.49	0.47
1:A:47:PRO:CB	1:A:48:PRO:HD2	2.45	0.47
1:A:229:ILE:HG13	1:A:230:HIS:N	2.29	0.47
1:A:149:ILE:O	1:A:152:ARG:HG3	2.14	0.47
1:B:296:SER:HA	5:B:1096:HOH:O	2.14	0.47
1:B:257:HIS:HD2	1:B:330:ASP:OD1	1.97	0.46
1:B:181:LYS:HE2	5:B:1726:HOH:O	2.15	0.46
1:A:316:ARG:HH21	1:A:342:ARG:CD	2.28	0.46
1:A:116:VAL:HG22	1:A:122:ILE:HG21	1.96	0.46
1:B:103:LEU:HD12	1:B:116:VAL:HG21	1.94	0.46
1:A:90:GLU:HG3	1:A:132:ILE:HG21	1.96	0.46
1:B:7:LEU:HG	1:B:343:TRP:CH2	2.51	0.46
1:B:68:ALA:HB2	5:B:1641:HOH:O	2.15	0.46
1:A:327:LEU:HB2	1:A:330:ASP:O	2.14	0.46
1:B:346:LYS:HA	5:B:1583:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:N	1:A:272:PRO:CD	2.78	0.46
1:A:162:GLU:OE2	1:A:162:GLU:HA	2.16	0.46
1:A:304:GLY:HA2	5:A:1208:HOH:O	2.15	0.45
1:A:123:MET:N	1:A:124:PRO:HD2	2.31	0.45
1:A:82:ASP:OD1	1:A:116:VAL:HA	2.16	0.45
1:A:15:TRP:CZ2	1:A:300:PRO:HD3	2.51	0.45
1:A:130:GLU:HG3	1:A:171:LEU:N	2.31	0.45
1:B:102:KCX:CX	1:B:104:TYR:CE2	2.99	0.45
1:B:315:VAL:HG23	1:B:344:SER:O	2.17	0.45
1:B:68:ALA:HB3	1:B:69:PRO:CD	2.39	0.45
1:A:85:ASP:O	1:A:88:GLU:N	2.42	0.45
1:A:80:LEU:HD22	1:A:125:VAL:HG11	1.99	0.45
1:B:123:MET:N	1:B:124:PRO:CD	2.79	0.45
1:A:123:MET:N	1:A:124:PRO:CD	2.79	0.44
1:B:242:PHE:CZ	1:B:244:ARG:CB	3.00	0.44
1:B:155[B]:ARG:HG2	5:B:1562:HOH:O	2.16	0.44
1:B:327:LEU:O	1:B:328:THR:C	2.55	0.44
1:B:127:GLU:HG3	1:B:168:LEU:HD21	1.99	0.44
1:B:82:ASP:OD2	1:B:117:THR:OG1	2.29	0.44
1:B:14:ASP:O	1:B:39:ALA:HA	2.17	0.44
1:A:212:VAL:HB	4:A:950:NCD:N1	2.32	0.44
1:A:11[A]:ARG:NE	1:A:312:ILE:CD1	2.80	0.44
1:B:289:GLN:HE21	1:B:289:GLN:H	1.63	0.44
1:A:59:ARG:HG3	1:A:74:PRO:HG2	1.99	0.44
1:B:10:ARG:HD3	1:B:307:VAL:HB	1.99	0.44
1:B:341:VAL:HG21	5:B:1475:HOH:O	2.18	0.44
1:A:257:HIS:ND1	1:A:330:ASP:OD2	2.39	0.44
1:A:162:GLU:N	1:A:163:PRO:CD	2.81	0.44
1:B:247:LEU:HG	1:B:278:TYR:CE1	2.53	0.44
4:A:950:NCD:C4	5:A:1446:HOH:O	2.66	0.43
1:A:66:VAL:CG1	1:A:70:HIS:HB2	2.48	0.43
1:A:107[A]:ASN:ND2	1:A:108:ALA:N	2.66	0.43
1:B:34:GLU:HG3	1:B:35:ILE:HG12	1.99	0.43
1:B:246:PHE:HB3	1:B:298:ASN:HB2	2.01	0.43
1:B:335:PHE:HA	5:B:1320:HOH:O	2.18	0.43
1:B:339:GLU:HG2	5:B:1582:HOH:O	2.18	0.43
1:A:192:GLU:CD	1:A:192:GLU:H	2.22	0.43
1:B:65:ALA:O	1:B:67:PRO:HD3	2.18	0.43
1:B:122:ILE:C	1:B:124:PRO:HD2	2.38	0.43
1:B:242:PHE:CE2	1:B:244:ARG:CB	3.01	0.43
1:B:19:LEU:HB3	1:B:25:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:OD1	1:A:208:ASN:HB2	2.19	0.43
1:B:70:HIS:N	1:B:70:HIS:CD2	2.86	0.42
1:B:257:HIS:HD2	1:B:330:ASP:CG	2.23	0.42
1:B:114:HIS:O	1:B:115:GLY:O	2.37	0.42
1:A:341:VAL:HG13	5:A:1621:HOH:O	2.19	0.42
1:A:142[A]:VAL:HG21	1:A:155[A]:ARG:HG3	2.00	0.42
1:B:341:VAL:HG12	1:B:342:ARG:N	2.32	0.42
1:A:105:PRO:HB2	1:A:143:THR:CG2	2.49	0.42
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.65	0.42
1:B:157:ILE:HG21	5:B:1701:HOH:O	2.17	0.42
1:B:52:VAL:O	1:B:56:VAL:HG23	2.18	0.42
1:B:317:GLU:O	1:B:319:GLN:N	2.53	0.42
1:B:144:HIS:HB3	1:B:147:ILE:HG13	2.01	0.42
1:A:320:GLN:HE21	1:A:320:GLN:HB3	1.55	0.42
1:A:177:HIS:CE1	1:A:223:PRO:HD3	2.55	0.42
1:A:123:MET:HB3	1:A:123:MET:HE2	1.47	0.42
1:A:155[B]:ARG:CG	1:A:155[B]:ARG:HH11	2.32	0.42
1:A:123:MET:O	1:A:127:GLU:HG3	2.20	0.42
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.88	0.42
1:B:123:MET:HE3	1:B:167:ARG:CZ	2.50	0.42
1:B:42:MET:HA	1:B:43:PRO:HD3	1.86	0.41
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.82	0.41
1:B:247:LEU:C	1:B:247:LEU:HD23	2.40	0.41
1:A:10:ARG:HD3	1:A:307:VAL:CG1	2.50	0.41
1:A:93:PHE:CD2	1:A:132:ILE:HD12	2.55	0.41
1:A:60[A]:GLN:HE21	1:A:60[A]:GLN:HB3	1.54	0.41
1:B:51:THR:HB	5:B:1634:HOH:O	2.21	0.41
1:B:319:GLN:CG	1:B:320:GLN:N	2.81	0.41
1:A:120:ASP:HA	1:A:123:MET:HG2	2.01	0.41
1:A:21:ASP:CA	1:A:25[A]:LEU:HB2	2.50	0.41
1:B:340:THR:O	1:B:340:THR:HG22	2.20	0.41
1:B:52:VAL:HG13	1:B:97:VAL:CG2	2.41	0.41
1:B:179:THR:HA	1:B:234:LEU:HD11	2.02	0.41
1:A:243:GLN:HG2	5:A:1618:HOH:O	2.19	0.41
1:A:19:LEU:HB3	1:A:25[B]:LEU:HD13	2.01	0.41
1:A:110:THR:HG21	1:A:115:GLY:HA3	2.03	0.41
4:B:411:NCD:N3	4:B:411:NCD:C4	2.78	0.41
1:B:44:ASN:HB3	1:B:104:TYR:CE1	2.56	0.41
1:B:129:MET:HE1	1:B:136:LEU:HD13	2.02	0.41
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.89	0.41
1:B:52:VAL:CG2	1:B:92:GLY:CA	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:KCX:NZ	1:B:104:TYR:CZ	2.89	0.41
1:B:162:GLU:HG3	1:B:166:GLN:CD	2.41	0.40
1:A:321:VAL:N	1:A:339:GLU:O	2.43	0.40
1:A:21:ASP:HA	1:A:25[B]:LEU:HB2	2.04	0.40
1:A:67:PRO:C	1:A:69:PRO:HD2	2.41	0.40
1:A:162:GLU:CB	1:A:163:PRO:HD3	2.51	0.40
1:A:176:GLU:O	1:A:177:HIS:C	2.58	0.40
1:A:10:ARG:HD3	1:A:307:VAL:HG12	2.02	0.40
1:A:162:GLU:CB	1:A:163:PRO:CD	2.99	0.40
1:A:319:GLN:O	1:A:340:THR:HA	2.22	0.40
1:B:10:ARG:O	1:B:11:ARG:C	2.59	0.40
1:B:158:GLU:H	1:B:158:GLU:HG3	1.33	0.40
1:B:19:LEU:HD13	1:B:29:VAL:HG12	2.02	0.40
1:B:199:THR:HB	1:B:200:PRO:HD2	2.03	0.40
1:A:70:HIS:CD2	1:A:70:HIS:H	2.39	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)
5:A:1316:HOH:O	5:A:1687:HOH:O[1_455]	2.19	0.01

## 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	351/347 (101%)	333 (95%)	16 (5%)	2 (1%)	30	12
1	B	337/347 (97%)	309 (92%)	23 (7%)	5 (2%)	13	2
All	All	688/694 (99%)	642 (93%)	39 (6%)	7 (1%)	21	4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	GLU
1	A	177	HIS
1	B	115	GLY
1	B	177	HIS
1	B	91[A]	ARG
1	B	91[B]	ARG
1	A	68	ALA

### 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	302/295 (102%)	275 (91%)	27 (9%)	12	2
1	B	291/295 (99%)	264 (91%)	27 (9%)	11	2
All	All	593/590 (100%)	539 (91%)	54 (9%)	13	2

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	11[A]	ARG
1	A	11[B]	ARG
1	A	35	ILE
1	A	60[A]	GLN
1	A	60[B]	GLN
1	A	91	ARG
1	A	120	ASP
1	A	125	VAL
1	A	131[A]	LYS
1	A	131[B]	LYS
1	A	146	ASP
1	A	155[A]	ARG
1	A	155[B]	ARG
1	A	158	GLU
1	A	162	GLU
1	A	167	ARG

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Mol	Chain	Res	Type
1	A	172	LYS
1	A	175	PHE
1	A	224	ILE
1	A	227	ARG
1	A	243	GLN
1	A	289	GLN
1	A	296	SER
1	A	312	ILE
1	A	341	VAL
1	A	344	SER
1	B	4	SER
1	B	88	GLU
1	B	89	LEU
1	B	91[A]	ARG
1	B	91[B]	ARG
1	B	107	ASN
1	B	113	SER
1	B	123	MET
1	B	128	ARG
1	B	146	ASP
1	B	158	GLU
1	B	159	SER
1	B	165	ARG
1	B	167	ARG
1	B	175	PHE
1	B	177	HIS
1	B	224	ILE
1	B	227	ARG
1	B	229	ILE
1	B	243	GLN
1	B	244	ARG
1	B	286	ASN
1	B	289	GLN
1	B	315	VAL
1	B	319	GLN
1	B	320	GLN
1	B	344	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS

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Mol	Chain	Res	Type
1	A	289	GLN
1	A	319	GLN
1	A	320	GLN
1	B	5	GLN
1	B	107	ASN
1	B	243	GLN
1	B	257	HIS
1	B	289	GLN
1	B	319	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	102	1,2	7,11,12	0.67	0	7,12,14	5.74	1 (14%)
1	KCX	B	102	1,2	7,11,12	0.59	0	7,12,14	6.04	1 (14%)

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	102	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	102	1,2	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	KCX	CE-NZ-CX	-15.77	105.64	123.49
1	A	102	KCX	CE-NZ-CX	-15.05	106.45	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	102	KCX	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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
3	ORO	A	410	-	4,11,11	6.54	3 (75%)	4,15,15	8.34	4 (100%)
4	NCD	A	950	-	5,11,11	1.16	1 (20%)	6,14,14	2.01	2 (33%)
4	NCD	B	411	2	5,11,11	0.83	0	6,14,14	2.22	3 (50%)

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
3	ORO	A	410	-	-	0/0/4/4	0/1/1/1
4	NCD	A	950	-	-	1/6/12/12	0/0/0/0
4	NCD	B	411	2	-	1/6/12/12	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	950	NCD	C5-C6	-2.09	1.50	1.53
3	A	410	ORO	C5-C6	2.09	1.46	1.40
3	A	410	ORO	C4-N3	4.08	1.40	1.33
3	A	410	ORO	C6-N1	12.22	1.51	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	ORO	C5-C6-N1	-12.78	107.48	122.39
3	A	410	ORO	C5-C4-N3	-5.28	117.66	124.05
4	B	411	NCD	O2-C2-N3	-3.29	117.67	123.30
4	A	950	NCD	O2-C2-N3	-3.20	117.82	123.30
4	B	411	NCD	C5-C6-C61	-2.17	106.90	111.55
4	B	411	NCD	N3-C2-N1	2.91	121.61	116.40
4	A	950	NCD	N3-C2-N1	2.92	121.62	116.40
3	A	410	ORO	C4-C5-C6	3.93	119.27	116.73
3	A	410	ORO	C4-N3-C2	8.47	122.53	114.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	411	NCD	N3-C2-N1-C6
4	A	950	NCD	N3-C2-N1-C6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	950	NCD	5	0
4	B	411	NCD	2	0

## 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	342/347 (98%)	-0.29	3 (0%) 85 88	13, 25, 51, 78	0
1	B	338/347 (97%)	0.02	9 (2%) 58 62	16, 31, 62, 92	0
All	All	680/694 (97%)	-0.13	12 (1%) 71 76	13, 28, 58, 92	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	ALA	3.8
1	B	113	SER	3.2
1	B	68	ALA	2.7
1	B	4	SER	2.7
1	B	319	GLN	2.6
1	A	109	THR	2.3
1	B	341	VAL	2.3
1	B	340	THR	2.2
1	B	6	VAL	2.2
1	B	69	PRO	2.1
1	A	4	SER	2.1
1	A	107[A]	ASN	2.1

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	B	102	12/13	0.89	0.13	-	20,27,32,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KCX	A	102	12/13	0.95	0.11	-	16,19,27,30	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NCD	A	950	12/12	0.78	0.28	5.64	37,45,71,77	0
3	ORO	A	410	11/11	0.97	0.09	0.69	17,21,39,100	0
4	NCD	B	411	12/12	0.91	0.09	0.20	24,30,40,48	0
2	ZN	B	400	1/1	0.98	0.06	-2.56	30,30,30,30	0
2	ZN	B	401	1/1	0.97	0.06	-4.99	35,35,35,35	0
2	ZN	A	401	1/1	1.00	0.04	-7.41	29,29,29,29	0
2	ZN	A	400	1/1	0.99	0.05	-11.50	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.