



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:01 am GMT

PDB ID : 2JBW  
Title : CRYSTAL STRUCTURE OF THE 2,6-DIHYDROXY-PSEUDO-OXYNICTINE HYDROLASE.  
Authors : Schleberger, C.; Sachelaru, P.; Brandsch, R.; Schulz, G.E.  
Deposited on : 2006-12-14  
Resolution : 2.10 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

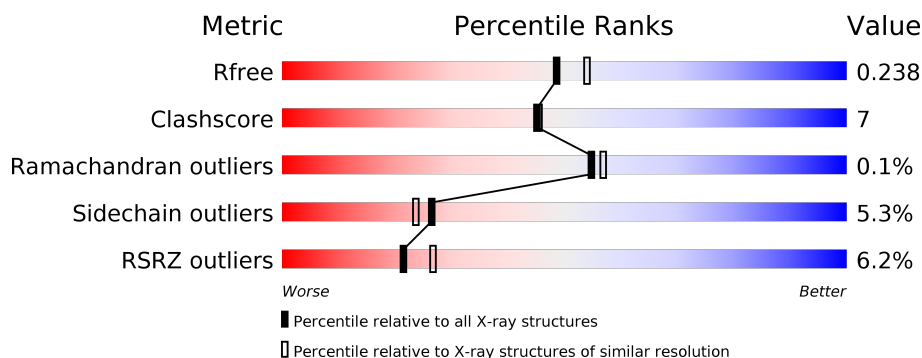
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	386	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	386	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• • 6%</div> </div> </div>
1	C	386	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>• 9%</div> </div> </div>
1	D	386	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12210 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 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	Se	0	0	1
			2828	1799	477	535	6	11			
1	B	361	Total	C	N	O	S	Se	0	0	1
			2827	1799	477	534	6	11			
1	C	352	Total	C	N	O	S	Se	0	0	1
			2761	1760	468	517	6	10			
1	D	360	Total	C	N	O	S	Se	0	0	1
			2826	1799	477	533	6	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ASP	LEU	CONFLICT	UNP Q93NG6
B	14	ASP	LEU	CONFLICT	UNP Q93NG6
C	14	ASP	LEU	CONFLICT	UNP Q93NG6
D	14	ASP	LEU	CONFLICT	UNP Q93NG6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

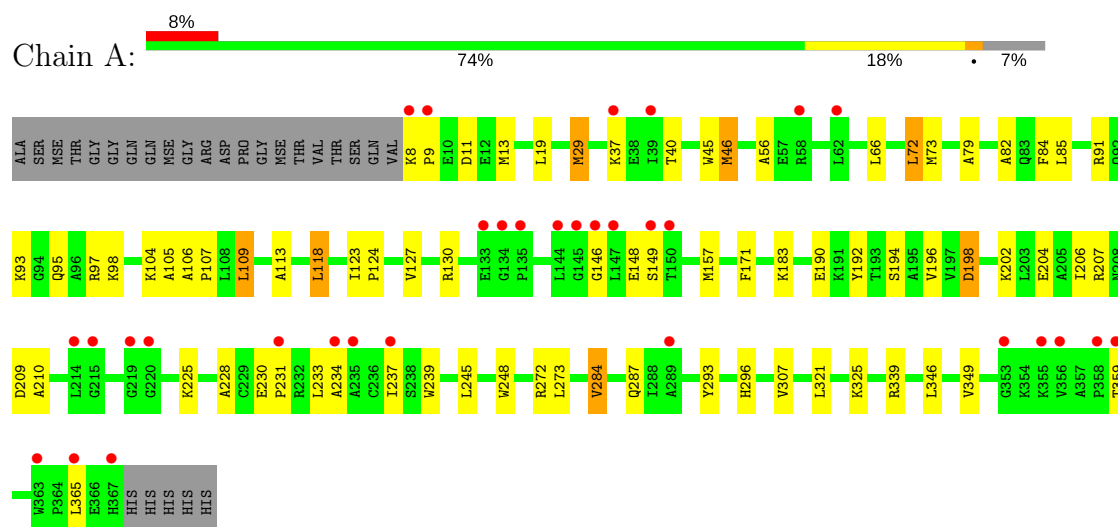
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total 103	O 103	0	0
3	B	160	Total 160	O 160	0	0
3	C	255	Total 255	O 255	0	0
3	D	446	Total 446	O 446	0	0

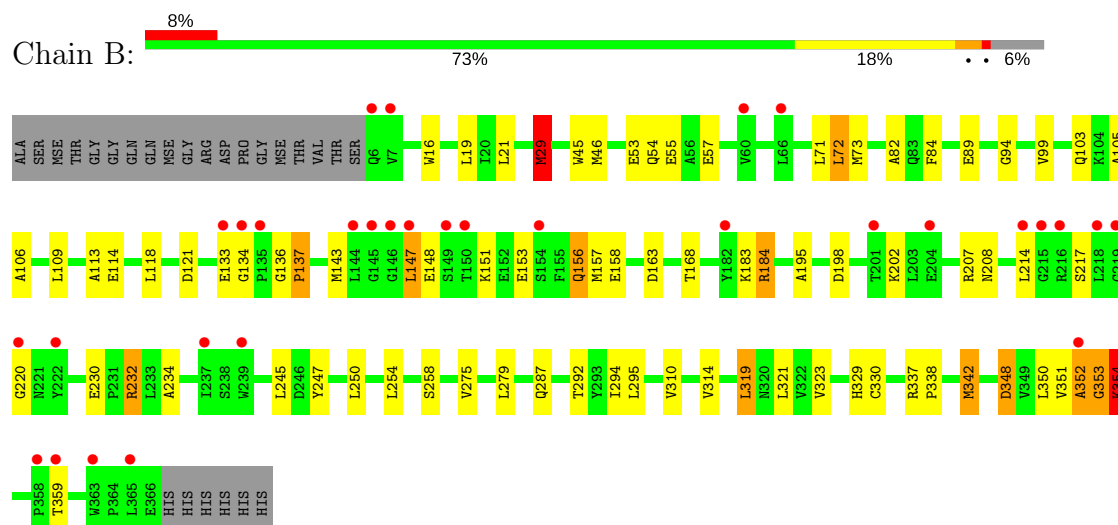
### 3 Residue-property plots

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

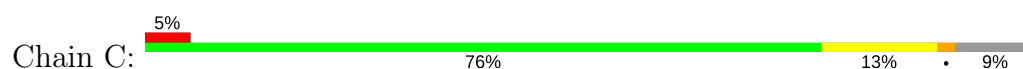
#### • Molecule 1: 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE

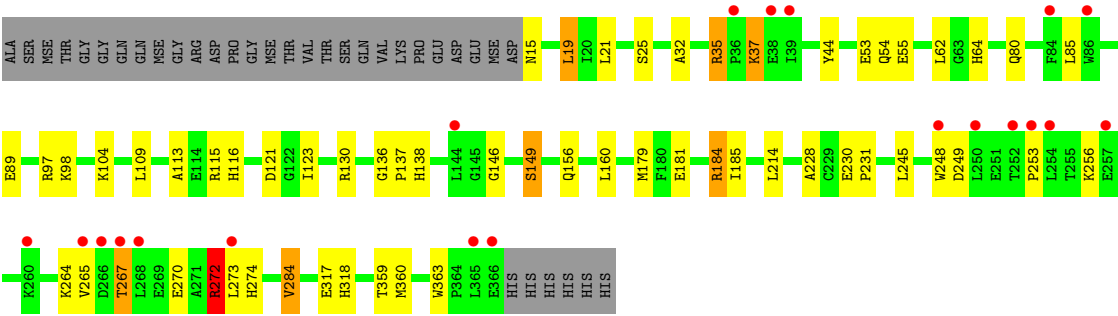


#### • Molecule 1: 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE

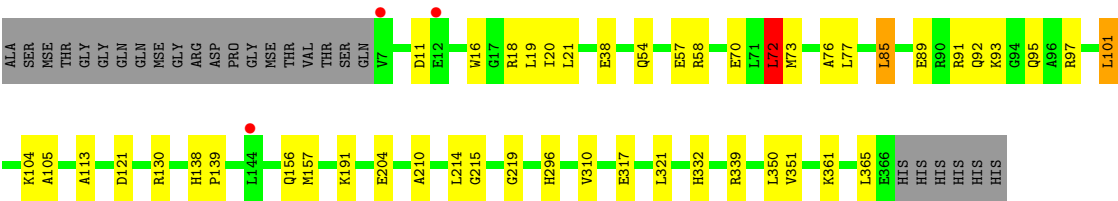
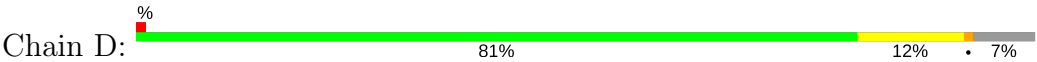


#### • Molecule 1: 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE





● Molecule 1: 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.57Å 57.02Å 152.70Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.10) 99.9 (29.77-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.17 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.181 , 0.238 0.181 , 0.238	Depositor DCC
$R_{free}$ test set	2580 reflections (2.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.93	13/2886 (0.5%)	0.69	2/3903 (0.1%)
1	B	1.25	21/2885 (0.7%)	0.77	5/3904 (0.1%)
1	C	0.72	0/2819	0.73	0/3815
1	D	0.98	2/2884 (0.1%)	0.86	5/3901 (0.1%)
All	All	0.99	36/11474 (0.3%)	0.77	12/15523 (0.1%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	LYS	CD-CE	37.57	2.45	1.51
1	B	353	GLY	N-CA	23.32	1.81	1.46
1	A	204	GLU	CD-OE2	16.64	1.44	1.25
1	A	198	ASP	CB-CG	14.79	1.82	1.51
1	B	114	GLU	CD-OE2	14.12	1.41	1.25
1	B	351	VAL	C-O	11.66	1.45	1.23
1	B	354	LYS	C-O	11.40	1.45	1.23
1	A	233	LEU	C-O	10.67	1.43	1.23
1	A	209	ASP	CB-CG	9.76	1.72	1.51
1	D	73	MSE	SE-CE	-9.04	1.42	1.95
1	A	204	GLU	CD-OE1	8.99	1.35	1.25
1	B	352	ALA	C-O	8.35	1.39	1.23
1	A	231	PRO	N-CD	7.99	1.59	1.47
1	A	231	PRO	C-O	7.78	1.38	1.23
1	B	234	ALA	CA-CB	7.65	1.68	1.52
1	A	206	ILE	C-O	7.38	1.37	1.23
1	A	209	ASP	CG-OD2	7.36	1.42	1.25
1	B	352	ALA	C-N	7.08	1.45	1.33
1	A	230	GLU	CG-CD	6.89	1.62	1.51
1	B	202	LYS	CE-NZ	6.79	1.66	1.49
1	A	194	SER	C-O	6.62	1.35	1.23
1	B	136	GLY	CA-C	6.50	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	ASN	CG-ND2	6.42	1.48	1.32
1	A	233	LEU	C-N	6.39	1.48	1.34
1	B	287	GLN	C-O	6.00	1.34	1.23
1	B	114	GLU	CD-OE1	5.99	1.32	1.25
1	B	133	GLU	C-O	5.93	1.34	1.23
1	B	133	GLU	C-N	5.89	1.43	1.33
1	B	348	ASP	CG-OD2	5.84	1.38	1.25
1	B	353	GLY	C-N	5.76	1.47	1.34
1	B	232	ARG	NE-CZ	5.62	1.40	1.33
1	D	76	ALA	CA-CB	5.38	1.63	1.52
1	B	351	VAL	CA-C	5.21	1.66	1.52
1	B	137	PRO	N-CD	5.14	1.55	1.47
1	A	230	GLU	CA-CB	5.13	1.65	1.53
1	B	287	GLN	C-N	5.04	1.45	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASP	CB-CG-OD2	7.88	125.40	118.30
1	D	72	LEU	CB-CG-CD1	6.58	122.18	111.00
1	D	157	MSE	CG-SE-CE	-6.51	84.58	98.90
1	B	352	ALA	N-CA-CB	6.40	119.06	110.10
1	B	184	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	58	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	354	LYS	CB-CA-C	-5.47	99.46	110.40
1	B	29	MSE	CG-SE-CE	-5.44	86.92	98.90
1	A	204	GLU	OE1-CD-OE2	5.38	129.75	123.30
1	D	339	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	85	LEU	CB-CG-CD1	5.15	119.75	111.00
1	B	351	VAL	CB-CA-C	-5.04	101.82	111.40

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	2828	0	2765	41	0
1	B	2827	0	2759	53	0
1	C	2761	0	2710	42	0
1	D	2826	0	2768	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	103	0	0	4	0
3	B	160	0	0	5	0
3	C	255	0	0	12	0
3	D	446	0	0	15	0
All	All	12210	0	11002	165	0

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 7.

All (165) 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:198:ASP:CB	1:A:198:ASP:CG	1.82	1.45
1:B:353:GLY:CA	1:B:353:GLY:N	1.81	1.42
1:A:13:MSE:HE1	3:A:2016:HOH:O	1.33	1.23
1:C:138:HIS:HD2	3:C:2165:HOH:O	1.22	1.22
1:B:143:MSE:HE1	1:B:158:GLU:CG	1.74	1.16
3:C:2130:HOH:O	1:D:70:GLU:HG3	1.59	1.03
1:B:143:MSE:HE1	1:B:158:GLU:HG2	1.36	1.03
1:B:143:MSE:HE1	1:B:158:GLU:HG3	1.44	0.99
1:D:138:HIS:HD2	3:D:2190:HOH:O	1.46	0.96
1:B:354:LYS:CE	1:B:354:LYS:CD	2.45	0.94
1:D:21:LEU:HD12	3:D:2409:HOH:O	1.70	0.90
1:D:138:HIS:CD2	3:D:2190:HOH:O	2.19	0.90
1:B:16:TRP:CZ3	1:B:29:MSE:HG2	2.15	0.82
1:C:53:GLU:OE2	1:C:104:LYS:NZ	2.13	0.81
1:D:54:GLN:NE2	3:D:2073:HOH:O	1.98	0.77
1:C:253:PRO:HA	1:C:256:LYS:HE2	1.65	0.77
1:A:157:MSE:HE3	1:A:239:TRP:CZ3	2.20	0.75
1:B:143:MSE:CE	1:B:158:GLU:HG2	2.16	0.75
1:C:37:LYS:H	1:C:37:LYS:HD3	1.51	0.74
1:C:273:LEU:HB3	3:C:2063:HOH:O	1.87	0.74
1:B:46:MSE:HE1	1:B:94:GLY:HA2	1.71	0.72
1:C:138:HIS:CD2	3:C:2165:HOH:O	2.09	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:HIS:HD2	3:D:2298:HOH:O	1.73	0.71
1:B:337:ARG:HB3	1:B:338:PRO:HD3	1.73	0.70
1:B:230:GLU:OE1	1:B:232:ARG:HG3	1.92	0.70
1:D:89:GLU:HG3	3:D:2049:HOH:O	1.90	0.70
1:A:157:MSE:HE3	1:A:239:TRP:CH2	2.26	0.69
1:B:16:TRP:CE3	1:B:29:MSE:HG2	2.27	0.69
1:D:92:GLN:HG3	3:D:2121:HOH:O	1.92	0.69
1:A:190:GLU:OE1	1:A:225:LYS:HE3	1.93	0.68
1:C:123:ILE:HG21	1:C:179:MSE:HE3	1.74	0.68
1:C:267:THR:HB	1:C:270:GLU:H	1.59	0.68
1:B:143:MSE:HE2	1:B:168:THR:HB	1.74	0.68
1:B:275:VAL:HG13	1:B:279:LEU:HD12	1.77	0.67
1:D:296:HIS:HE1	3:D:2376:HOH:O	1.79	0.65
1:A:171:PHE:CD1	1:A:196:VAL:HG21	2.31	0.65
1:C:37:LYS:H	1:C:37:LYS:CD	2.09	0.64
1:C:317:GLU:HG3	3:C:2221:HOH:O	1.97	0.64
1:C:318:HIS:HD2	3:C:2220:HOH:O	1.80	0.63
1:A:46:MSE:HE1	1:A:79:ALA:CB	2.29	0.62
1:B:183:LYS:HE2	3:B:2085:HOH:O	1.98	0.62
1:B:348:ASP:HA	1:B:352:ALA:HB3	1.82	0.62
1:D:21:LEU:O	1:D:156:GLN:HG3	2.00	0.62
1:A:13:MSE:CE	3:A:2016:HOH:O	2.11	0.60
1:D:11:ASP:OD1	3:D:2008:HOH:O	2.17	0.60
1:A:46:MSE:HE3	1:A:46:MSE:HA	1.84	0.60
1:C:116:HIS:HD2	3:C:2160:HOH:O	1.84	0.60
1:C:53:GLU:OE1	1:C:97:ARG:NH2	2.22	0.59
1:A:66:LEU:HD21	1:B:163:ASP:HB3	1.84	0.59
1:A:183:LYS:HE3	1:A:192:TYR:OH	2.03	0.59
1:D:317:GLU:HG2	3:D:2392:HOH:O	2.03	0.59
1:B:292:THR:HG22	1:B:294:ILE:CD1	2.33	0.59
1:C:253:PRO:CA	1:C:256:LYS:HE2	2.33	0.59
1:C:55:GLU:HG2	3:D:2417:HOH:O	2.01	0.58
1:A:9:PRO:O	1:A:13:MSE:HG3	2.03	0.58
1:A:105:ALA:O	1:A:109:LEU:HD13	2.03	0.58
1:A:46:MSE:HE1	1:A:79:ALA:HB2	1.85	0.58
1:B:53:GLU:O	1:B:57:GLU:HG3	2.03	0.58
1:A:13:MSE:HE3	1:A:85:LEU:HB2	1.84	0.58
1:D:18:ARG:HB2	1:D:332:HIS:HB3	1.86	0.58
1:C:32:ALA:HB2	1:C:44:TYR:CE2	2.39	0.57
1:B:295:LEU:CB	1:B:342:MSE:HE1	2.35	0.57
1:D:72:LEU:HB3	1:D:105:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:TRP:CD2	1:C:272:ARG:HG3	2.40	0.56
1:C:64:HIS:CE1	3:C:2043:HOH:O	2.59	0.56
1:C:184:ARG:HB3	1:C:264:LYS:HD2	1.88	0.56
1:B:72:LEU:HB3	1:B:105:ALA:HB2	1.87	0.56
1:C:115:ARG:NH2	3:C:2085:HOH:O	2.39	0.56
1:C:270:GLU:HA	1:C:273:LEU:HD12	1.88	0.56
1:B:73:MSE:HG2	1:B:109:LEU:HD11	1.87	0.55
1:B:310:VAL:HG23	1:B:314:VAL:CG2	2.36	0.55
1:B:310:VAL:HG23	1:B:314:VAL:HG21	1.89	0.54
1:C:228:ALA:CB	1:C:284:VAL:HG13	2.39	0.53
1:C:228:ALA:HB1	1:C:284:VAL:HG13	1.89	0.53
1:D:16:TRP:O	1:D:20:ILE:HG12	2.08	0.53
1:B:151:LYS:HE3	3:B:2052:HOH:O	2.08	0.53
1:A:72:LEU:HB3	1:A:105:ALA:HB2	1.91	0.53
1:B:19:LEU:CD2	1:B:29:MSE:HE1	2.39	0.52
1:B:319:LEU:HD22	1:B:321:LEU:HB2	1.91	0.52
1:B:153:GLU:O	1:B:153:GLU:HG2	2.08	0.52
1:A:207:ARG:HB2	1:A:210:ALA:HB3	1.91	0.52
1:B:19:LEU:HD23	1:B:29:MSE:HE1	1.92	0.51
1:C:113:ALA:HA	1:C:130:ARG:HG2	1.93	0.51
1:D:139:PRO:HB3	1:D:210:ALA:HB1	1.93	0.50
1:A:146:GLY:H	1:A:149:SER:HB2	1.76	0.50
1:B:106:ALA:HB1	1:B:113:ALA:HB3	1.94	0.50
1:A:113:ALA:HA	1:A:130:ARG:HG2	1.94	0.50
1:B:121:ASP:HB3	3:B:2049:HOH:O	2.11	0.50
1:A:198:ASP:CA	1:A:198:ASP:CG	2.75	0.49
1:D:214:LEU:C	1:D:214:LEU:HD23	2.33	0.49
1:C:185:ILE:HG23	1:C:274:HIS:CE1	2.47	0.49
1:B:147:LEU:HG	1:B:258:SER:HB3	1.95	0.49
1:C:116:HIS:HE1	3:C:2084:HOH:O	1.96	0.49
1:C:146:GLY:H	1:C:149:SER:HB3	1.78	0.49
1:D:77:LEU:HD12	3:D:2099:HOH:O	2.13	0.49
1:B:137:PRO:HG2	1:B:207:ARG:HG2	1.95	0.48
1:B:295:LEU:HB2	1:B:342:MSE:HE1	1.95	0.48
1:A:118:LEU:HD22	1:A:127:VAL:HG21	1.94	0.48
1:A:234:ALA:HB2	3:A:2058:HOH:O	2.12	0.48
1:C:32:ALA:O	1:C:35:ARG:HG3	2.14	0.48
1:A:19:LEU:HD22	1:A:29:MSE:HE1	1.97	0.47
1:A:307:VAL:HG13	1:A:321:LEU:HD21	1.97	0.47
1:B:295:LEU:HB2	1:B:342:MSE:CE	2.45	0.47
1:A:284:VAL:HG22	1:A:287:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ARG:O	1:D:95:GLN:HG2	2.15	0.46
1:B:245:LEU:HD13	1:B:247:TYR:CE1	2.51	0.46
1:B:147:LEU:HB2	3:B:2058:HOH:O	2.15	0.46
1:D:214:LEU:HD23	1:D:215:GLY:N	2.30	0.46
1:B:310:VAL:CG2	1:B:314:VAL:HG21	2.46	0.46
1:C:80:GLN:HG2	1:C:98:LYS:HD3	1.97	0.46
1:D:139:PRO:HG2	1:D:351:VAL:HG22	1.97	0.45
1:B:217:SER:O	1:B:220:GLY:N	2.49	0.45
1:C:156:GLN:HE22	1:C:160:LEU:HD11	1.80	0.45
1:D:97:ARG:HG3	1:D:101:LEU:HD22	1.98	0.45
1:C:21:LEU:O	1:C:156:GLN:HG3	2.16	0.45
1:D:57:GLU:OE2	1:D:104:LYS:NZ	2.49	0.45
1:B:352:ALA:C	1:B:353:GLY:CA	2.79	0.45
1:A:248:TRP:CD2	1:A:272:ARG:HG3	2.51	0.45
1:B:275:VAL:HG13	1:B:279:LEU:CD1	2.45	0.44
1:A:106:ALA:HA	1:A:109:LEU:HD22	1.98	0.44
1:D:361:LYS:HE2	3:D:2402:HOH:O	2.16	0.44
1:B:21:LEU:O	1:B:156:GLN:HG2	2.17	0.44
1:C:121:ASP:O	1:C:123:ILE:HD12	2.17	0.44
1:C:214:LEU:HD23	1:C:214:LEU:C	2.37	0.44
1:B:55:GLU:HB3	1:B:71:LEU:HD13	1.99	0.44
1:B:89:GLU:CD	1:B:89:GLU:H	2.21	0.44
1:C:360:MSE:SE	1:C:363:TRP:HD1	2.51	0.44
1:A:157:MSE:HE1	1:A:339:ARG:HD3	2.00	0.43
1:A:123:ILE:HA	1:A:124:PRO:HD2	1.90	0.43
1:B:292:THR:HG22	1:B:294:ILE:HD12	2.01	0.43
1:B:184:ARG:NH1	1:D:121:ASP:O	2.50	0.43
1:A:95:GLN:HE22	1:A:98:LYS:HZ1	1.67	0.43
1:D:215:GLY:HA3	1:D:219:GLY:O	2.19	0.43
1:C:185:ILE:CG2	1:C:274:HIS:CE1	3.01	0.42
1:D:204:GLU:HG2	3:D:2275:HOH:O	2.19	0.42
1:A:45:TRP:HB2	1:A:82:ALA:HB2	2.01	0.42
1:D:191:LYS:HE2	3:D:2169:HOH:O	2.19	0.42
1:A:296:HIS:HD2	3:A:2060:HOH:O	2.03	0.42
1:B:99:VAL:O	1:B:103:GLN:HG3	2.20	0.42
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.90	0.42
1:C:230:GLU:HA	1:C:231:PRO:HD2	1.85	0.42
1:B:245:LEU:HG	1:B:275:VAL:HG12	2.02	0.42
1:C:15:ASN:O	1:C:19:LEU:HD22	2.20	0.42
1:B:45:TRP:HB2	1:B:82:ALA:HB2	2.02	0.42
1:C:98:LYS:HB3	1:C:98:LYS:HE2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LYS:HD3	1:C:37:LYS:N	2.28	0.42
1:C:136:GLY:HA3	1:C:137:PRO:HA	1.77	0.41
1:A:8:LYS:HG2	1:A:11:ASP:OD2	2.20	0.41
1:B:295:LEU:HD22	1:B:342:MSE:HE1	2.03	0.41
1:D:89:GLU:OE1	1:D:93:LYS:HE2	2.21	0.41
1:A:228:ALA:CB	1:A:284:VAL:HG13	2.50	0.41
1:A:237:ILE:HD11	1:A:346:LEU:HG	2.02	0.41
1:B:195:ALA:O	1:B:198:ASP:HB2	2.20	0.41
1:B:134:GLY:N	3:B:2054:HOH:O	2.43	0.41
1:B:156:GLN:HG3	1:B:157:MSE:N	2.36	0.41
1:D:113:ALA:HA	1:D:130:ARG:HG2	2.03	0.41
1:A:104:LYS:O	1:A:107:PRO:HD2	2.21	0.41
1:A:56:ALA:HB3	1:A:72:LEU:HD13	2.02	0.40
1:B:329:HIS:O	1:B:330:CYS:HB2	2.21	0.40
1:A:157:MSE:CE	1:A:239:TRP:CH2	2.99	0.40
1:A:346:LEU:HA	1:A:349:VAL:HG22	2.02	0.40
1:C:54:GLN:NE2	3:C:2033:HOH:O	2.49	0.40
1:A:202:LYS:HE2	1:A:202:LYS:HB3	1.91	0.40
1:A:237:ILE:HG12	1:A:293:TYR:HB3	2.02	0.40
1:C:64:HIS:ND1	3:C:2043:HOH:O	2.37	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	358/386 (93%)	347 (97%)	11 (3%)	0	100	100
1	B	359/386 (93%)	349 (97%)	10 (3%)	0	100	100
1	C	350/386 (91%)	337 (96%)	12 (3%)	1 (0%)	44	44
1	D	358/386 (93%)	351 (98%)	7 (2%)	0	100	100
All	All	1425/1544 (92%)	1384 (97%)	40 (3%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	272	ARG

### 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	299/307 (97%)	280 (94%)	19 (6%)	20	17
1	B	298/307 (97%)	281 (94%)	17 (6%)	24	21
1	C	291/307 (95%)	273 (94%)	18 (6%)	21	18
1	D	299/307 (97%)	290 (97%)	9 (3%)	46	49
All	All	1187/1228 (97%)	1124 (95%)	63 (5%)	26	24

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MSE
1	A	37	LYS
1	A	40	THR
1	A	46	MSE
1	A	72	LEU
1	A	73	MSE
1	A	84	PHE
1	A	91	ARG
1	A	93	LYS
1	A	97	ARG
1	A	109	LEU
1	A	118	LEU
1	A	148	GLU
1	A	245	LEU
1	A	273	LEU
1	A	284	VAL
1	A	325	LYS
1	A	359	THR
1	A	365	LEU

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Mol	Chain	Res	Type
1	B	29	MSE
1	B	54	GLN
1	B	72	LEU
1	B	84	PHE
1	B	118	LEU
1	B	147	LEU
1	B	148	GLU
1	B	156	GLN
1	B	214	LEU
1	B	250	LEU
1	B	254	LEU
1	B	319	LEU
1	B	323	VAL
1	B	342	MSE
1	B	350	LEU
1	B	354	LYS
1	B	359	THR
1	C	19	LEU
1	C	25	SER
1	C	35	ARG
1	C	37	LYS
1	C	62	LEU
1	C	85	LEU
1	C	89	GLU
1	C	109	LEU
1	C	149	SER
1	C	181	GLU
1	C	184	ARG
1	C	245	LEU
1	C	249	ASP
1	C	265	VAL
1	C	267	THR
1	C	272	ARG
1	C	284	VAL
1	C	359	THR
1	D	19	LEU
1	D	38	GLU
1	D	72	LEU
1	D	85	LEU
1	D	101	LEU
1	D	310	VAL
1	D	321	LEU

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Mol	Chain	Res	Type
1	D	350	LEU
1	D	365	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	103	GLN
1	A	156	GLN
1	A	296	HIS
1	B	54	GLN
1	B	287	GLN
1	C	54	GLN
1	C	116	HIS
1	C	138	HIS
1	C	274	HIS
1	C	287	GLN
1	C	296	HIS
1	C	318	HIS
1	D	138	HIS
1	D	296	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

### 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	349/386 (90%)	0.43	32 (9%) 10 12	32, 50, 80, 130	0
1	B	350/386 (90%)	0.45	31 (8%) 10 13	28, 49, 85, 115	0
1	C	342/386 (88%)	0.12	20 (5%) 24 30	12, 31, 67, 76	0
1	D	349/386 (90%)	-0.36	3 (0%) 84 86	10, 19, 37, 61	0
All	All	1390/1544 (90%)	0.16	86 (6%) 21 27	10, 39, 75, 130	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	THR	5.9
1	A	353	GLY	5.7
1	D	7	VAL	5.5
1	C	267	THR	5.4
1	C	86	TRP	5.3
1	A	365	LEU	5.0
1	A	134	GLY	4.5
1	B	144	LEU	4.3
1	B	237	ILE	4.0
1	C	273	LEU	3.8
1	B	7	VAL	3.7
1	A	214	LEU	3.6
1	B	363	TRP	3.6
1	C	366	GLU	3.6
1	A	37	LYS	3.5
1	A	367	HIS	3.5
1	B	219	GLY	3.4
1	B	145	GLY	3.3
1	C	365	LEU	3.3
1	C	248	TRP	3.3
1	A	149	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	216	ARG	3.1
1	B	218	LEU	3.1
1	B	133	GLU	3.1
1	B	147	LEU	3.1
1	C	268	LEU	3.1
1	B	146	GLY	3.1
1	A	144	LEU	3.0
1	A	237	ILE	3.0
1	B	215	GLY	2.9
1	B	149	SER	2.9
1	B	154	SER	2.9
1	B	6	GLN	2.9
1	C	39	ILE	2.8
1	B	135	PRO	2.8
1	C	260	LYS	2.8
1	B	214	LEU	2.8
1	A	215	GLY	2.8
1	B	134	GLY	2.8
1	A	235	ALA	2.8
1	A	363	TRP	2.8
1	A	219	GLY	2.8
1	B	66	LEU	2.8
1	B	201	THR	2.7
1	A	289	ALA	2.7
1	C	144	LEU	2.7
1	A	359	THR	2.7
1	A	135	PRO	2.6
1	B	358	PRO	2.6
1	C	84	PHE	2.6
1	A	9	PRO	2.6
1	C	253	PRO	2.6
1	C	36	PRO	2.6
1	B	60	VAL	2.6
1	B	182	TYR	2.6
1	C	266	ASP	2.5
1	A	8	LYS	2.5
1	A	231	PRO	2.5
1	A	356	VAL	2.5
1	B	352	ALA	2.5
1	A	150	THR	2.5
1	B	365	LEU	2.5
1	A	145	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	257	GLU	2.4
1	A	234	ALA	2.4
1	A	147	LEU	2.4
1	A	220	GLY	2.4
1	C	38	GLU	2.4
1	D	12	GLU	2.4
1	A	133	GLU	2.4
1	B	222	TYR	2.4
1	C	250	LEU	2.3
1	A	358	PRO	2.3
1	B	239	TRP	2.3
1	B	359	THR	2.3
1	A	39	ILE	2.3
1	B	150	THR	2.3
1	A	146	GLY	2.3
1	A	58	ARG	2.2
1	A	62	LEU	2.2
1	B	204	GLU	2.2
1	B	220	GLY	2.1
1	A	355	LYS	2.1
1	C	265	VAL	2.0
1	C	254	LEU	2.0
1	D	144	LEU	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 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
2	NA	C	1367	1/1	0.91	0.09	-0.67	36,36,36,36	0
2	NA	A	1368	1/1	0.93	0.10	-1.60	53,53,53,53	0
2	NA	B	1367	1/1	0.90	0.11	-2.15	56,56,56,56	0
2	NA	D	1367	1/1	0.97	0.05	-2.71	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.