



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:56 AM UTC

PDB ID : 2JBW / pdb_00002jbw
Title : Crystal Structure of the 2,6-dihydroxy-pseudo-oxynicotine 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

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

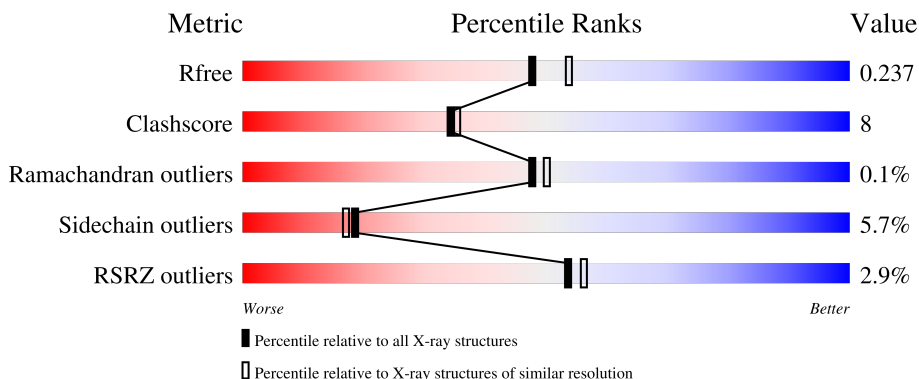
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

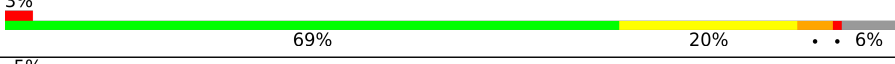
The reported resolution of this entry is 2.10 Å.

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	386	
1	B	386	
1	C	386	
1	D	386	

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 (CCD ID: NA) (formula: Na).

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

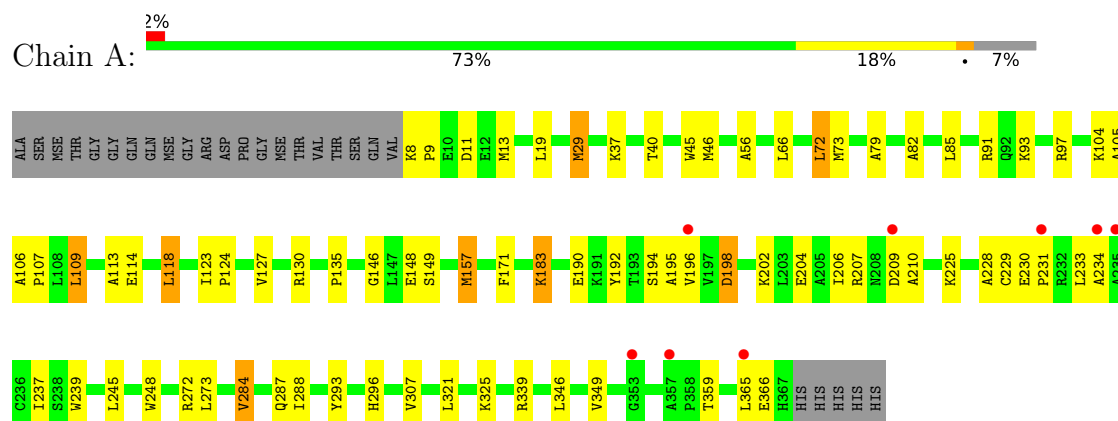
- Molecule 3 is water.

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

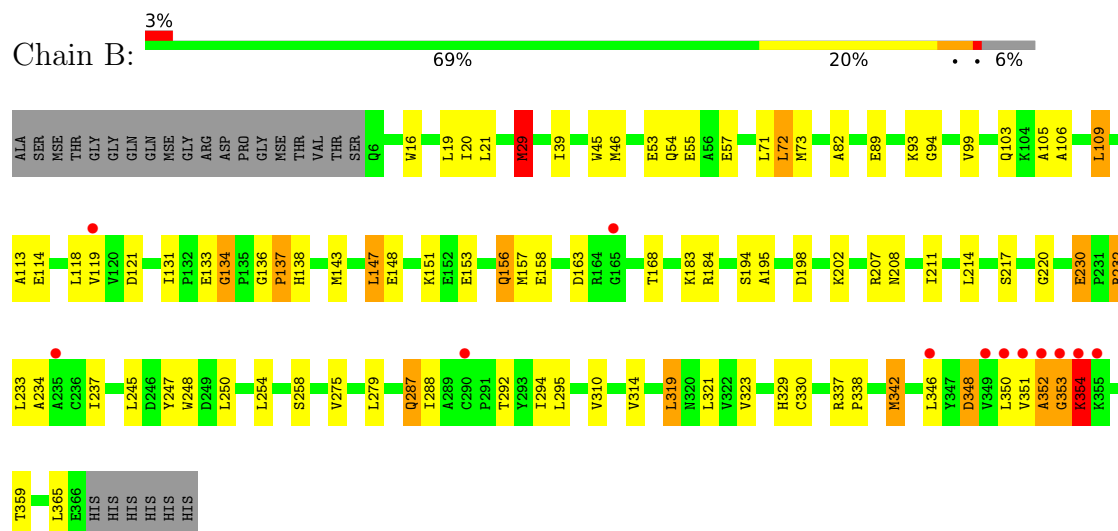
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

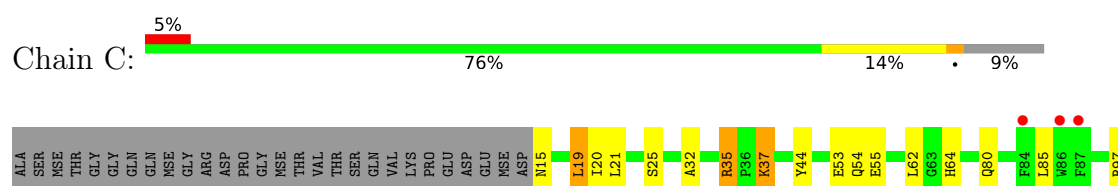
• Molecule 1: 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE

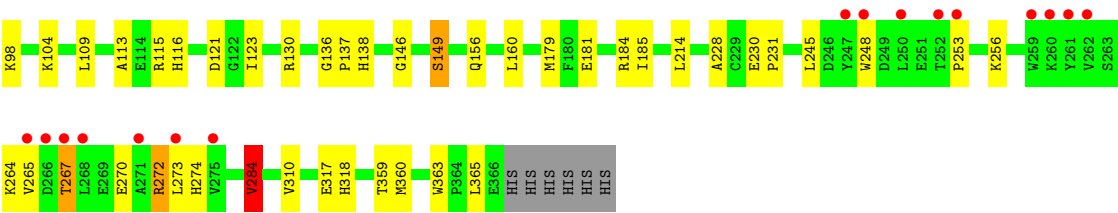


• Molecule 1: 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE

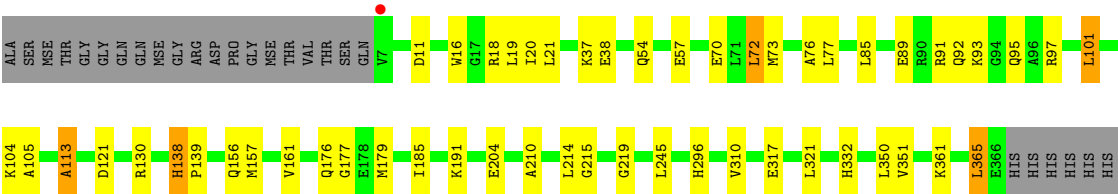
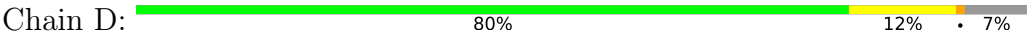


• Molecule 1: 2,6-DIHYDROXY-PSEUDO-OXYNICOTINE HYDROLASE





● 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, α , β , γ	90.57Å 57.02Å 152.70Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.10) 99.8 (30.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.238 0.181 , 0.237	Depositor DCC
R_{free} test set	2580 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.11	22/2886 (0.8%)	0.96	2/3903 (0.1%)
1	B	1.45	35/2885 (1.2%)	1.08	17/3904 (0.4%)
1	C	0.89	1/2819 (0.0%)	1.01	2/3815 (0.1%)
1	D	1.19	7/2884 (0.2%)	1.06	3/3901 (0.1%)
All	All	1.18	65/11474 (0.6%)	1.03	24/15523 (0.2%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	LYS	CD-CE	30.91	2.45	1.52
1	B	353	GLY	N-CA	24.99	1.81	1.45
1	B	351	VAL	C-O	20.53	1.45	1.23
1	D	73	MSE	SE-CE	-17.78	1.42	1.95
1	B	354	LYS	C-O	16.90	1.45	1.24
1	A	233	LEU	C-O	16.41	1.43	1.23
1	A	206	ILE	C-O	13.06	1.37	1.24
1	B	352	ALA	C-O	12.81	1.39	1.24
1	A	198	ASP	CB-CG	12.30	1.82	1.52
1	A	231	PRO	C-O	11.44	1.38	1.24
1	B	351	VAL	CA-C	10.04	1.66	1.52
1	A	233	LEU	C-N	9.87	1.48	1.33
1	B	353	GLY	C-N	9.81	1.47	1.33
1	A	204	GLU	CD-OE2	9.79	1.44	1.25
1	A	194	SER	C-O	9.47	1.35	1.24
1	B	287	GLN	C-N	9.33	1.45	1.33
1	B	352	ALA	C-N	9.29	1.45	1.33
1	A	209	ASP	CG-OD2	8.91	1.42	1.25
1	B	234	ALA	CA-CB	8.88	1.68	1.53
1	A	230	GLU	CA-CB	8.85	1.65	1.52
1	B	133	GLU	C-O	8.82	1.34	1.23
1	A	209	ASP	C-N	8.59	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	GLU	CD-OE2	8.33	1.41	1.25
1	B	352	ALA	CA-C	-8.16	1.41	1.52
1	B	287	GLN	C-O	8.12	1.34	1.24
1	A	209	ASP	CB-CG	8.08	1.72	1.52
1	A	231	PRO	N-CD	8.06	1.59	1.47
1	B	208	ASN	CG-ND2	7.45	1.48	1.33
1	A	157	MSE	SE-CE	-7.34	1.73	1.95
1	B	233	LEU	C-O	7.32	1.32	1.24
1	A	135	PRO	C-O	7.30	1.32	1.23
1	A	230	GLU	C-O	7.26	1.31	1.24
1	B	136	GLY	CA-C	7.23	1.62	1.51
1	B	194	SER	C-N	7.20	1.43	1.33
1	B	348	ASP	CG-OD2	7.07	1.38	1.25
1	B	133	GLU	C-N	6.82	1.43	1.33
1	B	208	ASN	C-O	6.80	1.32	1.24
1	B	354	LYS	CA-C	-6.79	1.44	1.52
1	B	131	ILE	CA-CB	6.76	1.59	1.54
1	B	346	LEU	CA-C	6.75	1.61	1.52
1	B	119	VAL	C-O	6.75	1.31	1.24
1	A	366	GLU	C-N	-6.67	1.24	1.33
1	B	232	ARG	NE-CZ	6.64	1.40	1.33
1	A	229	CYS	C-N	6.49	1.39	1.33
1	B	351	VAL	C-N	-6.36	1.25	1.33
1	B	136	GLY	N-CA	6.36	1.53	1.44
1	D	76	ALA	CA-CB	6.30	1.63	1.53
1	B	365	LEU	C-N	-6.21	1.24	1.33
1	B	234	ALA	N-CA	6.19	1.54	1.46
1	C	365	LEU	C-N	-6.15	1.24	1.33
1	A	288	ILE	C-N	5.96	1.42	1.33
1	B	119	VAL	C-N	5.92	1.41	1.33
1	A	206	ILE	C-N	5.78	1.41	1.33
1	D	73	MSE	CA-C	5.64	1.59	1.52
1	B	202	LYS	CE-NZ	5.56	1.66	1.49
1	D	185	ILE	CA-CB	5.56	1.60	1.54
1	B	353	GLY	C-O	5.48	1.31	1.23
1	D	365	LEU	C-N	-5.37	1.25	1.33
1	D	179	MSE	SE-CE	5.37	2.11	1.95
1	A	204	GLU	CD-OE1	5.36	1.35	1.25
1	A	195	ALA	CA-C	-5.33	1.46	1.52
1	A	135	PRO	C-N	5.32	1.41	1.33
1	D	113	ALA	CA-CB	5.28	1.60	1.53
1	B	137	PRO	N-CD	5.14	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	ILE	CA-C	5.12	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	GLY	CA-C-N	8.77	128.82	119.78
1	B	134	GLY	C-N-CA	8.77	128.82	119.78
1	B	351	VAL	CB-CA-C	-8.46	101.82	111.80
1	B	352	ALA	N-CA-C	7.87	120.85	111.33
1	B	230	GLU	CA-C-N	7.13	127.74	119.47
1	B	230	GLU	C-N-CA	7.13	127.74	119.47
1	B	352	ALA	CA-C-O	6.54	127.69	120.63
1	D	157	MSE	CG-SE-CE	-6.52	84.58	98.92
1	B	354	LYS	CB-CA-C	-6.45	99.46	110.22
1	B	352	ALA	N-CA-CB	6.00	119.06	110.06
1	A	135	PRO	O-C-N	5.66	129.88	122.86
1	B	29	MSE	CG-SE-CE	-5.46	86.92	98.92
1	C	20	ILE	N-CA-C	5.37	116.00	110.36
1	B	138	HIS	CA-C-N	-5.32	114.47	119.85
1	B	138	HIS	C-N-CA	-5.32	114.47	119.85
1	C	284	VAL	CB-CA-C	5.32	115.63	110.63
1	B	233	LEU	CA-C-N	-5.08	113.83	122.56
1	B	233	LEU	C-N-CA	-5.08	113.83	122.56
1	B	133	GLU	O-C-N	5.08	129.08	122.89
1	B	353	GLY	CA-C-O	5.07	126.03	119.44
1	A	209	ASP	CA-CB-CG	-5.04	107.56	112.60
1	D	138	HIS	CA-C-N	-5.02	115.39	120.21
1	D	138	HIS	C-N-CA	-5.02	115.39	120.21
1	B	194	SER	O-C-N	5.02	127.51	122.09

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	40	0
1	B	2827	0	2759	55	0
1	C	2761	0	2710	42	0
1	D	2826	0	2768	33	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	168	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 8.

All (168) 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	1.49
1:B:353:GLY:N	1:B:353:GLY:CA	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
1:B:143:MSE:HE1	1:B:158:GLU:HG2	1.36	1.03
3:C:2130:HOH:O	1:D:70:GLU:HG3	1.59	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:CD	1:B:354:LYS:CE	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:HD3	1:C:37:LYS:H	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:D:214:LEU:C	1:D:214:LEU:HD23	2.33	0.54
1:A:198:ASP:CG	1:A:198:ASP:CA	2.75	0.54
1:B:310:VAL:HG23	1:B:314:VAL:HG21	1.89	0.54
1:B:352:ALA:C	1:B:353:GLY:CA	2.79	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: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:C:214:LEU:C	1:C:214:LEU:HD23	2.37	0.49
1:B:89:GLU:H	1:B:89:GLU:CD	2.21	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:55:GLU:HB3	1:B:71:LEU:HD13	1.99	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:184:ARG:NH1	1:D:121:ASP:O	2.50	0.43
1:B:292:THR:HG22	1:B:294:ILE:HD12	2.01	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:HE2	1:C:98:LYS:HB3	1.87	0.42
1:C:37:LYS:HD3	1:C:37:LYS:N	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD	1:D:93:LYS:HE2	2.44	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:248:TRP:CD1	1:B:248:TRP:C	2.96	0.41
1:A:104:LYS:O	1:A:107:PRO:HD2	2.21	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:B:287:GLN:O	1:B:288:ILE:C	2.64	0.41
1:D:176:GLN:O	1:D:177:GLY:C	2.64	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 [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	358/386 (93%)	347 (97%)	11 (3%)	0	100	100
1	B	359/386 (93%)	349 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	350/386 (91%)	337 (96%)	12 (3%)	1 (0%)	36	36
1	D	358/386 (93%)	351 (98%)	7 (2%)	0	100	100
All	All	1425/1544 (92%)	1384 (97%)	40 (3%)	1 (0%)	48	50

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%)	16	14
1	B	298/307 (97%)	276 (93%)	22 (7%)	13	10
1	C	291/307 (95%)	276 (95%)	15 (5%)	21	20
1	D	299/307 (97%)	287 (96%)	12 (4%)	28	29
All	All	1187/1228 (97%)	1119 (94%)	68 (6%)	18	17

All (68) 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	72	LEU
1	A	73	MSE
1	A	91	ARG
1	A	93	LYS
1	A	97	ARG
1	A	109	LEU
1	A	114	GLU
1	A	118	LEU

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Mol	Chain	Res	Type
1	A	148	GLU
1	A	183	LYS
1	A	245	LEU
1	A	273	LEU
1	A	284	VAL
1	A	325	LYS
1	A	359	THR
1	A	365	LEU
1	B	20	ILE
1	B	29	MSE
1	B	39	ILE
1	B	54	GLN
1	B	72	LEU
1	B	93	LYS
1	B	109	LEU
1	B	118	LEU
1	B	147	LEU
1	B	148	GLU
1	B	156	GLN
1	B	211	ILE
1	B	214	LEU
1	B	237	ILE
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	109	LEU
1	C	149	SER
1	C	181	GLU
1	C	245	LEU
1	C	265	VAL
1	C	267	THR

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Mol	Chain	Res	Type
1	C	284	VAL
1	C	310	VAL
1	C	359	THR
1	D	19	LEU
1	D	37	LYS
1	D	38	GLU
1	D	72	LEU
1	D	85	LEU
1	D	101	LEU
1	D	161	VAL
1	D	245	LEU
1	D	310	VAL
1	D	321	LEU
1	D	350	LEU
1	D	365	LEU

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	95	GLN
1	A	103	GLN
1	A	156	GLN
1	A	296	HIS
1	B	54	GLN
1	B	83	GLN
1	B	156	GLN
1	B	287	GLN
1	B	332	HIS
1	C	54	GLN
1	C	116	HIS
1	C	138	HIS
1	C	274	HIS
1	C	287	GLN
1	C	299	HIS
1	C	318	HIS
1	D	92	GLN
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 oligosaccharides 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	349/386 (90%)	0.34	8 (2%) 61 64	32, 50, 80, 130	0
1	B	350/386 (90%)	0.37	12 (3%) 48 50	28, 49, 85, 115	0
1	C	342/386 (88%)	0.08	19 (5%) 30 32	12, 31, 67, 76	0
1	D	349/386 (90%)	-0.59	1 (0%) 90 91	10, 19, 37, 61	0
All	All	1390/1544 (90%)	0.05	40 (2%) 53 56	10, 39, 75, 130	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	ALA	3.9
1	C	268	LEU	3.9
1	C	267	THR	3.6
1	C	261	TYR	3.2
1	C	248	TRP	3.2
1	B	119	VAL	3.1
1	B	351	VAL	3.1
1	C	262	VAL	3.1
1	B	353	GLY	3.0
1	A	209	ASP	3.0
1	A	234	ALA	3.0
1	A	353	GLY	2.9
1	A	235	ALA	2.9
1	B	235	ALA	2.9
1	A	365	LEU	2.9
1	A	231	PRO	2.9
1	B	349	VAL	2.8
1	C	273	LEU	2.7
1	A	357	ALA	2.7
1	A	196	VAL	2.6
1	C	260	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	259	TRP	2.6
1	C	265	VAL	2.4
1	B	290	CYS	2.4
1	B	346	LEU	2.3
1	B	354	LYS	2.3
1	C	86	TRP	2.3
1	C	266	ASP	2.3
1	C	87	PHE	2.2
1	C	253	PRO	2.2
1	C	275	VAL	2.2
1	B	355	LYS	2.2
1	B	350	LEU	2.2
1	C	252	THR	2.2
1	C	84	PHE	2.1
1	C	271	ALA	2.1
1	C	247	TYR	2.1
1	B	165	GLY	2.0
1	D	7	VAL	2.0
1	C	250	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 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	NA	C	1367	1/1	0.90	0.06	36,36,36,36	0
2	NA	A	1368	1/1	0.93	0.06	53,53,53,53	0
2	NA	B	1367	1/1	0.94	0.06	56,56,56,56	0
2	NA	D	1367	1/1	0.97	0.05	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.