



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 10:46 pm GMT

PDB ID : 5FYI
Title : Crystal structure of human JMJD2A in complex with pyruvate
Authors : Nowak, R.; Kopec, J.; Johansson, C.; Szykowska, A.; von Delft, F.; Arrow-smith, C.H.; Bountra, C.; Edwards, A.; Oppermann, U.
Deposited on : 2016-03-07
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

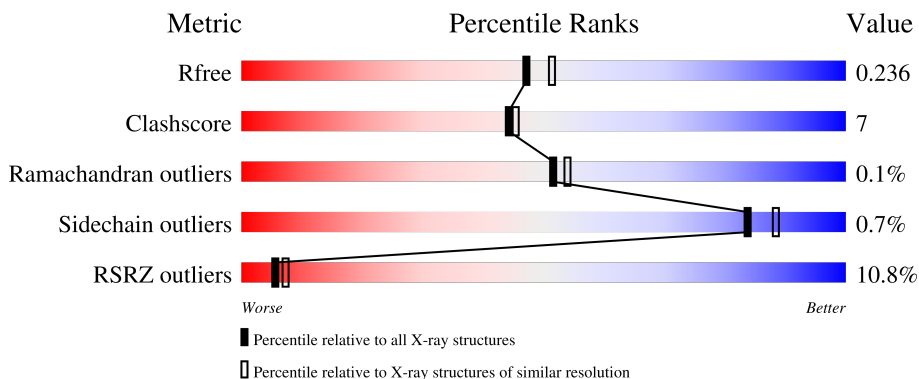
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	381	 9% (red), 80% (green), 12% (yellow), 8% (grey)
1	B	381	 10% (red), 77% (green), 13% (yellow), 10% (grey)

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
3	PYR	A	1356	-	-	-	X
3	PYR	B	1355	-	-	-	X
5	EDO	A	1358	-	-	X	-
5	EDO	B	1357	-	-	X	-
5	EDO	B	1364	-	-	-	X
7	1KA	B	1365	-	X	-	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 6036 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 LYSINE-SPECIFIC DEMETHYLASE 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2844	1844	468	517	15	0	5	0
1	B	344	2756	1791	455	494	16	0	1	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP O75164
A	-20	HIS	-	expression tag	UNP O75164
A	-19	HIS	-	expression tag	UNP O75164
A	-18	HIS	-	expression tag	UNP O75164
A	-17	HIS	-	expression tag	UNP O75164
A	-16	HIS	-	expression tag	UNP O75164
A	-15	HIS	-	expression tag	UNP O75164
A	-14	SER	-	expression tag	UNP O75164
A	-13	SER	-	expression tag	UNP O75164
A	-12	GLY	-	expression tag	UNP O75164
A	-11	VAL	-	expression tag	UNP O75164
A	-10	ASP	-	expression tag	UNP O75164
A	-9	LEU	-	expression tag	UNP O75164
A	-8	GLY	-	expression tag	UNP O75164
A	-7	THR	-	expression tag	UNP O75164
A	-6	GLU	-	expression tag	UNP O75164
A	-5	ASN	-	expression tag	UNP O75164
A	-4	LEU	-	expression tag	UNP O75164
A	-3	TYR	-	expression tag	UNP O75164
A	-2	PHE	-	expression tag	UNP O75164
A	-1	GLN	-	expression tag	UNP O75164
A	0	SER	-	expression tag	UNP O75164
B	-21	MET	-	expression tag	UNP O75164
B	-20	HIS	-	expression tag	UNP O75164
B	-19	HIS	-	expression tag	UNP O75164

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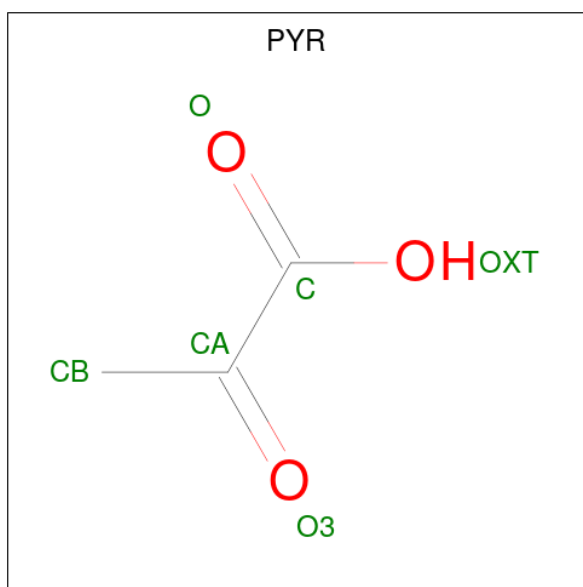
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP O75164
B	-17	HIS	-	expression tag	UNP O75164
B	-16	HIS	-	expression tag	UNP O75164
B	-15	HIS	-	expression tag	UNP O75164
B	-14	SER	-	expression tag	UNP O75164
B	-13	SER	-	expression tag	UNP O75164
B	-12	GLY	-	expression tag	UNP O75164
B	-11	VAL	-	expression tag	UNP O75164
B	-10	ASP	-	expression tag	UNP O75164
B	-9	LEU	-	expression tag	UNP O75164
B	-8	GLY	-	expression tag	UNP O75164
B	-7	THR	-	expression tag	UNP O75164
B	-6	GLU	-	expression tag	UNP O75164
B	-5	ASN	-	expression tag	UNP O75164
B	-4	LEU	-	expression tag	UNP O75164
B	-3	TYR	-	expression tag	UNP O75164
B	-2	PHE	-	expression tag	UNP O75164
B	-1	GLN	-	expression tag	UNP O75164
B	0	SER	-	expression tag	UNP O75164

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

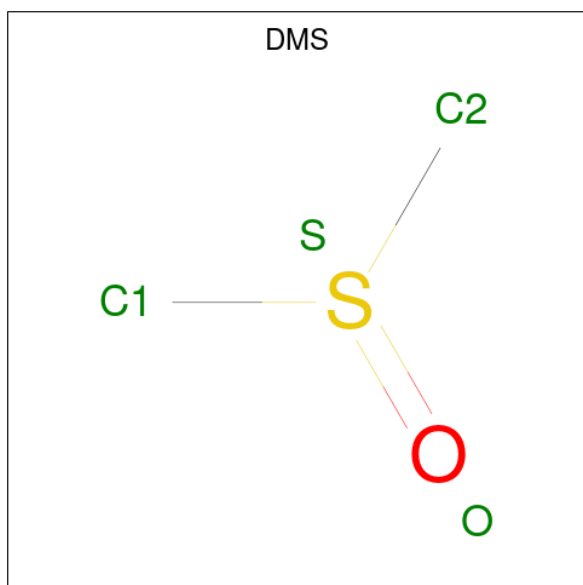
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0
2	B	1	Total Ni 1 1	0	0

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: C₃H₄O₃).



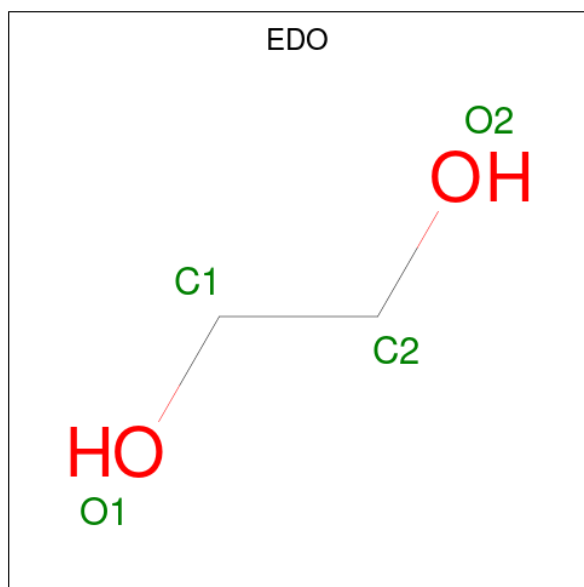
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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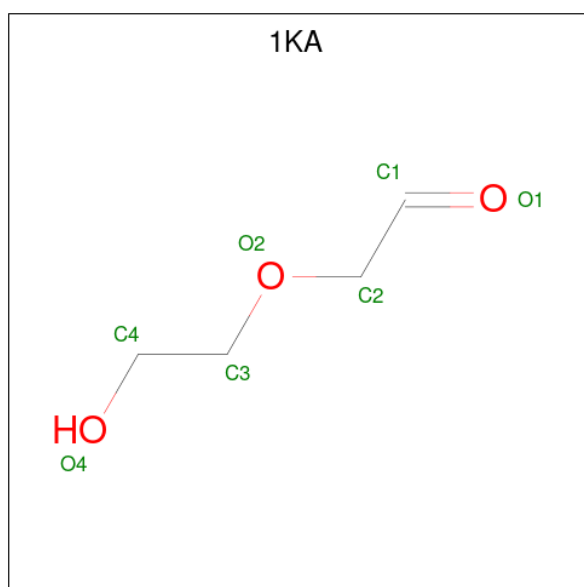
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0

- Molecule 7 is (2-hydroxyethoxy)acetaldehyde (three-letter code: 1KA) (formula: C₄H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		

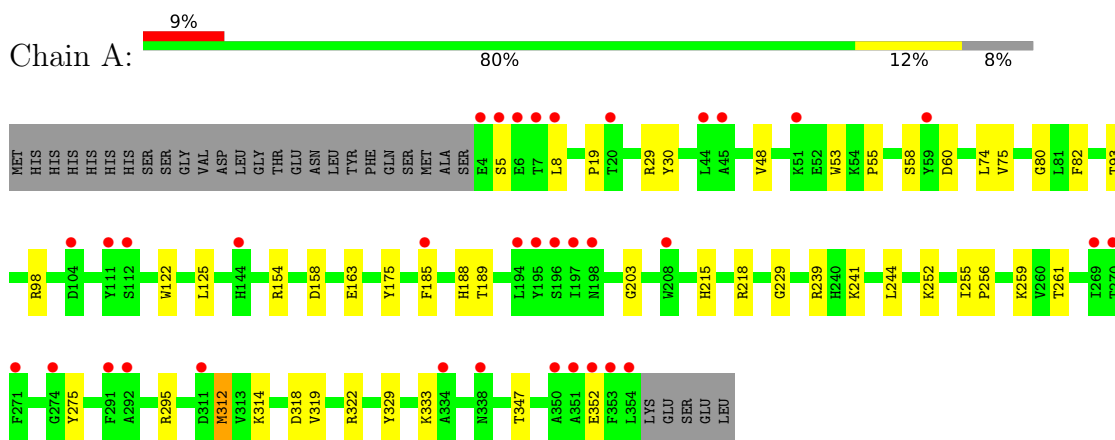
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	159	Total	O	0	0
			159	159		
8	B	166	Total	O	0	0
			166	166		

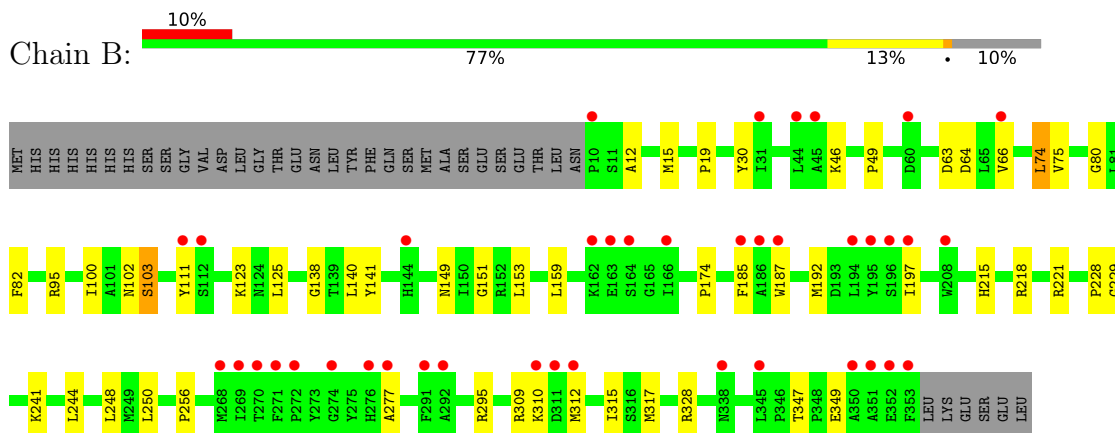
3 Residue-property plots [i](#)

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: LYSINE-SPECIFIC DEMETHYLASE 4A



- Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 4A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.45Å 148.83Å 57.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.10 29.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.77-2.10) 95.7 (29.77-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.197 , 0.236 0.199 , 0.236	Depositor DCC
R_{free} test set	2457 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6036	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, 1KA, NI, EDO, ZN, DMS

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	0.40	0/2940	0.54	1/3993 (0.0%)
1	B	0.42	0/2843	0.55	1/3863 (0.0%)
All	All	0.41	0/5783	0.55	2/7856 (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	74	LEU	CA-CB-CG	-5.53	102.59	115.30
1	A	74	LEU	CA-CB-CG	-5.37	102.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2844	0	2702	34	0
1	B	2756	0	2602	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
4	A	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	6	2	0
5	A	36	0	54	9	0
5	B	32	0	48	11	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	7	0	8	1	0
8	A	159	0	0	5	0
8	B	166	0	0	6	0
All	All	6036	0	5426	73	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 (73) 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:317[B]:MET:SD	1:B:317[B]:MET:N	2.41	0.92
1:B:277:ALA:HB1	5:B:1357:EDO:H21	1.56	0.88
1:A:93:THR:OG1	8:A:2020:HOH:O	2.01	0.78
1:A:239:ARG:HG2	5:A:1358:EDO:H12	1.71	0.73
1:B:248:LEU:HB2	5:B:1358:EDO:H21	1.71	0.70
1:A:163:GLU:HG3	1:A:319:VAL:HG21	1.75	0.69
1:A:203:GLY:O	8:A:2093:HOH:O	2.12	0.67
1:A:252:LYS:NZ	1:B:15:MET:SD	2.68	0.67
1:A:58:SER:OG	1:A:60:ASP:OD2	2.14	0.66
1:B:111:TYR:OH	8:B:2062:HOH:O	2.12	0.65
1:A:189:THR:H	5:A:1358:EDO:H11	1.62	0.65
1:B:49:PRO:O	8:B:2020:HOH:O	2.16	0.63
1:A:19:PRO:HB3	1:A:30:TYR:CZ	2.35	0.62
1:B:309:ARG:HD2	1:B:312:MET:HE2	1.85	0.57
1:B:151:GLY:HA2	1:B:174:PRO:HG3	1.86	0.57
1:A:241[A]:LYS:NZ	8:A:2087:HOH:O	2.38	0.56
1:B:100:ILE:O	1:B:103:SER:HB3	2.06	0.56
1:B:12:ALA:HB3	7:B:1365:1KA:H7	1.88	0.55
1:A:29:ARG:NE	1:A:352:GLU:OE2	2.39	0.55
1:B:244:LEU:HD22	5:B:1357:EDO:H11	1.88	0.55
1:A:188:HIS:CD2	1:A:241[B]:LYS:HE2	2.43	0.54
1:A:218[A]:ARG:HD2	1:A:255:ILE:HD13	1.90	0.52
1:A:5:SER:HA	1:A:8:LEU:HD12	1.92	0.52
1:A:322:ARG:HG3	1:A:329:TYR:CE1	2.45	0.51
1:A:19:PRO:HD2	1:A:48:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HG2	5:A:1358:EDO:C1	2.41	0.50
1:A:229:GLY:H	4:A:1357:DMS:H21	1.78	0.49
1:B:19:PRO:HB3	1:B:30:TYR:CZ	2.48	0.49
1:B:46:LYS:NZ	5:B:1363:EDO:H22	2.26	0.49
1:B:218:ARG:HG2	1:B:221:ARG:NH2	2.27	0.49
1:B:328:ARG:NE	8:B:2155:HOH:O	2.45	0.48
1:A:80:GLY:HA2	5:A:1359:EDO:H11	1.94	0.48
1:B:141:TYR:CE2	1:B:149:ASN:HA	2.48	0.48
1:A:189:THR:OG1	5:A:1358:EDO:H11	2.14	0.48
1:B:295:ARG:HB2	1:B:347:THR:HA	1.95	0.48
1:B:228:PRO:HD2	4:B:1356:DMS:H21	1.95	0.47
1:B:63:ASP:HB3	1:B:95:ARG:HB2	1.96	0.47
1:B:185:PHE:HB2	5:B:1364:EDO:H11	1.96	0.47
1:A:185:PHE:HB2	5:A:1365:EDO:H22	1.96	0.46
1:B:80:GLY:HA2	5:B:1358:EDO:H11	1.97	0.46
1:A:75:VAL:HG11	1:A:125:LEU:HG	1.98	0.46
1:B:64:ASP:OD1	1:B:95:ARG:NH2	2.43	0.45
1:B:215:HIS:CD2	1:B:256:PRO:HG2	2.51	0.45
1:A:295:ARG:HB2	1:A:347:THR:HA	1.98	0.45
1:B:102:ASN:HD22	5:B:1361:EDO:H21	1.81	0.45
1:B:349:GLU:OE2	8:B:2165:HOH:O	2.20	0.45
1:A:259:LYS:HB2	8:A:2095:HOH:O	2.16	0.44
1:B:66:VAL:O	8:B:2027:HOH:O	2.20	0.44
1:B:187:TRP:CZ2	1:B:250:LEU:HD11	2.53	0.44
1:A:98:ARG:NH1	8:A:2043:HOH:O	2.26	0.43
1:A:53:TRP:CZ3	1:A:55:PRO:HD3	2.54	0.43
1:A:154:ARG:HA	1:A:158:ASP:OD2	2.18	0.43
1:B:123:LYS:O	8:B:2069:HOH:O	2.21	0.43
1:B:82:PHE:HB2	1:B:244:LEU:HB2	2.01	0.43
1:A:318[B]:ASP:OD2	1:A:333:LYS:NZ	2.41	0.43
1:B:244:LEU:HD22	5:B:1357:EDO:C1	2.47	0.42
1:A:312:MET:CE	1:A:314:LYS:HB2	2.49	0.42
1:B:241:LYS:HD3	5:B:1364:EDO:H12	2.01	0.42
1:A:229:GLY:H	4:A:1357:DMS:C2	2.32	0.42
1:A:82:PHE:HB2	1:A:244:LEU:HB2	2.01	0.42
1:B:192:MET:HG3	1:B:315:ILE:HB	2.02	0.42
1:A:261:THR:HG21	5:A:1362:EDO:H12	2.02	0.42
1:A:215:HIS:CD2	1:A:256:PRO:HG2	2.55	0.41
1:B:153:LEU:HD11	1:B:197:ILE:HG21	2.02	0.41
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.82	0.41
1:A:275:TYR:CZ	5:A:1358:EDO:H21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TRP:HB3	5:A:1359:EDO:H22	2.01	0.41
1:B:75:VAL:HG11	1:B:125:LEU:HG	2.02	0.41
1:B:229:GLY:H	4:B:1356:DMS:C2	2.32	0.41
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.84	0.40
1:B:244:LEU:HD22	5:B:1357:EDO:H22	2.02	0.40
1:B:46:LYS:HZ3	5:B:1363:EDO:H22	1.86	0.40
1:B:138:GLY:O	1:B:174:PRO:HB2	2.20	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	354/381 (93%)	348 (98%)	6 (2%)	0	100	100
1	B	343/381 (90%)	337 (98%)	5 (2%)	1 (0%)	41	41
All	All	697/762 (92%)	685 (98%)	11 (2%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	LYS

5.3.2 Protein sidechains [i](#)

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	294/335 (88%)	292 (99%)	2 (1%)	84	88
1	B	279/335 (83%)	277 (99%)	2 (1%)	84	88
All	All	573/670 (86%)	569 (99%)	4 (1%)	84	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	TYR
1	A	312	MET
1	B	74	LEU
1	B	103	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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
5	EDO	B	1359	-	3,3,3	0.56	0	2,2,2	0.31	0
5	EDO	A	1359	-	3,3,3	0.42	0	2,2,2	0.51	0
3	PYR	B	1354	2	5,5,5	1.12	1 (20%)	3,6,6	0.85	0
4	DMS	B	1356	-	3,3,3	0.59	0	3,3,3	0.73	0
5	EDO	A	3001	-	3,3,3	0.49	0	2,2,2	0.26	0
4	DMS	A	1357	-	3,3,3	0.58	0	3,3,3	0.62	0
5	EDO	B	1357	-	3,3,3	0.42	0	2,2,2	0.28	0
5	EDO	A	1363	-	3,3,3	0.53	0	2,2,2	0.16	0
3	PYR	A	1356	-	5,5,5	0.92	0	3,6,6	0.89	0
5	EDO	A	1364	-	3,3,3	0.52	0	2,2,2	0.25	0
5	EDO	B	1360	-	3,3,3	0.70	0	2,2,2	0.21	0
5	EDO	A	1360	-	3,3,3	0.47	0	2,2,2	0.41	0
5	EDO	A	1365	-	3,3,3	0.55	0	2,2,2	0.08	0
5	EDO	B	1362	-	3,3,3	0.67	0	2,2,2	0.17	0
5	EDO	B	1361	-	3,3,3	0.53	0	2,2,2	0.19	0
5	EDO	B	1364	-	3,3,3	0.64	0	2,2,2	0.22	0
5	EDO	A	1362	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	A	1361	-	3,3,3	0.43	0	2,2,2	0.40	0
3	PYR	B	1355	-	5,5,5	0.95	0	3,6,6	0.87	0
7	1KA	B	1365	-	6,6,6	2.06	2 (33%)	5,5,5	2.88	1 (20%)
5	EDO	B	1358	-	3,3,3	0.43	0	2,2,2	0.37	0
3	PYR	A	1355	2	5,5,5	1.14	0	3,6,6	0.73	0
5	EDO	A	1358	-	3,3,3	0.55	0	2,2,2	0.35	0
5	EDO	B	1363	-	3,3,3	0.43	0	2,2,2	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1359	-	-	0/1/1/1	-
5	EDO	A	1359	-	-	0/1/1/1	-
3	PYR	B	1354	2	-	3/4/4/4	-
5	EDO	A	3001	-	-	0/1/1/1	-
5	EDO	B	1357	-	-	1/1/1/1	-
5	EDO	A	1363	-	-	0/1/1/1	-
3	PYR	A	1356	-	-	0/4/4/4	-
5	EDO	A	1364	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1360	-	-	1/1/1/1	-
5	EDO	A	1360	-	-	0/1/1/1	-
5	EDO	A	1365	-	-	1/1/1/1	-
5	EDO	B	1362	-	-	1/1/1/1	-
5	EDO	B	1361	-	-	0/1/1/1	-
5	EDO	B	1364	-	-	0/1/1/1	-
5	EDO	A	1362	-	-	0/1/1/1	-
5	EDO	A	1361	-	-	1/1/1/1	-
3	PYR	B	1355	-	-	0/4/4/4	-
7	1KA	B	1365	-	-	3/3/4/4	-
5	EDO	B	1358	-	-	1/1/1/1	-
3	PYR	A	1355	2	-	3/4/4/4	-
5	EDO	A	1358	-	-	0/1/1/1	-
5	EDO	B	1363	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1365	1KA	O1-C1	4.48	1.45	1.19
3	B	1354	PYR	O-C	2.14	1.28	1.22
7	B	1365	1KA	C3-C4	2.12	1.60	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1365	1KA	O1-C1-C2	-6.39	107.11	126.39

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1355	PYR	O-C-CA-CB
3	A	1355	PYR	OXT-C-CA-CB
3	B	1354	PYR	O-C-CA-CB
3	B	1354	PYR	OXT-C-CA-CB
5	B	1357	EDO	O1-C1-C2-O2
7	B	1365	1KA	O2-C3-C4-O4
5	A	1365	EDO	O1-C1-C2-O2
7	B	1365	1KA	C1-C2-O2-C3
5	B	1358	EDO	O1-C1-C2-O2
5	B	1362	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	1360	EDO	O1-C1-C2-O2
7	B	1365	1KA	C4-C3-O2-C2
5	A	1361	EDO	O1-C1-C2-O2
3	A	1355	PYR	OXT-C-CA-O3
3	B	1354	PYR	OXT-C-CA-O3

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1359	EDO	2	0
4	B	1356	DMS	2	0
4	A	1357	DMS	2	0
5	B	1357	EDO	4	0
5	A	1365	EDO	1	0
5	B	1361	EDO	1	0
5	B	1364	EDO	2	0
5	A	1362	EDO	1	0
7	B	1365	1KA	1	0
5	B	1358	EDO	2	0
5	A	1358	EDO	5	0
5	B	1363	EDO	2	0

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	351/381 (92%)	0.54	35 (9%) 7 9	27, 45, 71, 90	0
1	B	344/381 (90%)	0.61	40 (11%) 4 6	28, 45, 67, 87	0
All	All	695/762 (91%)	0.57	75 (10%) 5 7	27, 45, 70, 90	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	PHE	8.6
1	A	8	LEU	5.5
1	A	7	THR	5.5
1	A	354	LEU	5.4
1	B	311	ASP	5.3
1	B	166	ILE	5.0
1	B	351	ALA	4.8
1	A	311	ASP	4.4
1	A	269	ILE	4.3
1	B	162	LYS	4.0
1	A	5	SER	4.0
1	A	6	GLU	4.0
1	A	351	ALA	3.9
1	A	270	THR	3.9
1	B	269	ILE	3.9
1	B	112	SER	3.8
1	A	291	PHE	3.7
1	A	197	ILE	3.6
1	B	195	TYR	3.6
1	B	45	ALA	3.6
1	A	4	GLU	3.5
1	B	163	GLU	3.5
1	B	270	THR	3.4
1	A	195	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	196	SER	3.4
1	A	51	LYS	3.3
1	A	144	HIS	3.2
1	B	350	ALA	3.2
1	B	44	LEU	3.1
1	B	353	PHE	3.1
1	B	194	LEU	3.1
1	B	310	LYS	3.1
1	B	271	PHE	3.0
1	B	345	LEU	3.0
1	B	352	GLU	3.0
1	A	111	TYR	2.9
1	B	31	ILE	2.9
1	B	268	MET	2.9
1	B	196	SER	2.9
1	B	312	MET	2.8
1	B	208	TRP	2.8
1	B	197	ILE	2.8
1	A	194	LEU	2.7
1	A	271	PHE	2.7
1	A	352	GLU	2.6
1	B	60	ASP	2.6
1	B	291	PHE	2.6
1	A	112	SER	2.5
1	A	350	ALA	2.5
1	B	164	SER	2.5
1	B	338	ASN	2.5
1	B	10	PRO	2.4
1	A	104	ASP	2.4
1	A	185	PHE	2.4
1	A	44	LEU	2.4
1	B	111	TYR	2.4
1	B	144	HIS	2.4
1	B	277	ALA	2.3
1	A	208	TRP	2.3
1	B	185	PHE	2.2
1	B	187	TRP	2.2
1	A	198	ASN	2.2
1	A	20	THR	2.2
1	A	338	ASN	2.1
1	A	292	ALA	2.1
1	B	276	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	2.1
1	B	292	ALA	2.1
1	A	274	GLY	2.1
1	B	274	GLY	2.1
1	A	334	ALA	2.0
1	B	66	VAL	2.0
1	B	186	ALA	2.0
1	B	272	PRO	2.0
1	A	59	TYR	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 monosaccharides 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(\AA^2)	Q<0.9
5	EDO	B	1364	4/4	0.38	0.66	54,56,59,66	0
5	EDO	A	3001	4/4	0.64	0.29	68,71,73,80	0
3	PYR	A	1356	6/6	0.67	0.64	45,46,49,51	6
5	EDO	B	1360	4/4	0.71	0.35	42,50,51,57	0
5	EDO	A	1365	4/4	0.72	0.37	56,57,59,62	0
5	EDO	B	1361	4/4	0.75	0.19	58,66,71,72	0
3	PYR	B	1355	6/6	0.76	0.64	43,46,49,50	6
7	1KA	B	1365	7/7	0.78	0.21	57,64,66,66	0
5	EDO	A	1362	4/4	0.81	0.43	53,64,66,66	0
5	EDO	B	1362	4/4	0.85	0.28	41,44,53,62	0
5	EDO	A	1360	4/4	0.85	0.44	50,52,62,67	0
5	EDO	A	1363	4/4	0.85	0.46	53,56,60,63	0
5	EDO	A	1361	4/4	0.90	0.36	39,39,47,60	0
5	EDO	A	1364	4/4	0.90	0.20	55,61,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PYR	A	1355	6/6	0.90	0.26	33,39,43,44	6
5	EDO	A	1358	4/4	0.91	0.21	38,41,43,46	0
5	EDO	B	1363	4/4	0.92	0.28	49,54,59,59	0
5	EDO	B	1359	4/4	0.92	0.22	37,43,45,54	0
5	EDO	B	1358	4/4	0.92	0.24	46,50,53,67	0
5	EDO	B	1357	4/4	0.94	0.20	35,35,37,47	0
5	EDO	A	1359	4/4	0.95	0.25	39,42,42,45	0
3	PYR	B	1354	6/6	0.96	0.19	29,37,41,43	0
4	DMS	A	1357	4/4	0.96	0.14	42,52,54,56	0
4	DMS	B	1356	4/4	0.96	0.13	51,54,58,58	0
6	ZN	A	3000	1/1	0.99	0.06	34,34,34,34	0
6	ZN	B	502	1/1	0.99	0.06	40,40,40,40	0
2	NI	B	501	1/1	0.99	0.12	42,42,42,42	0
2	NI	A	501	1/1	1.00	0.10	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.