



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:30 PM UTC

PDB ID : 5M0I / pdb_00005m0i
Title : Crystal structure of the nuclear complex with She2p and the ASH1 mRNA
E3-localization element
Authors : Edelman, F.T.; Janowski, R.; Niessing, D.
Deposited on : 2016-10-05
Resolution : 2.41 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:

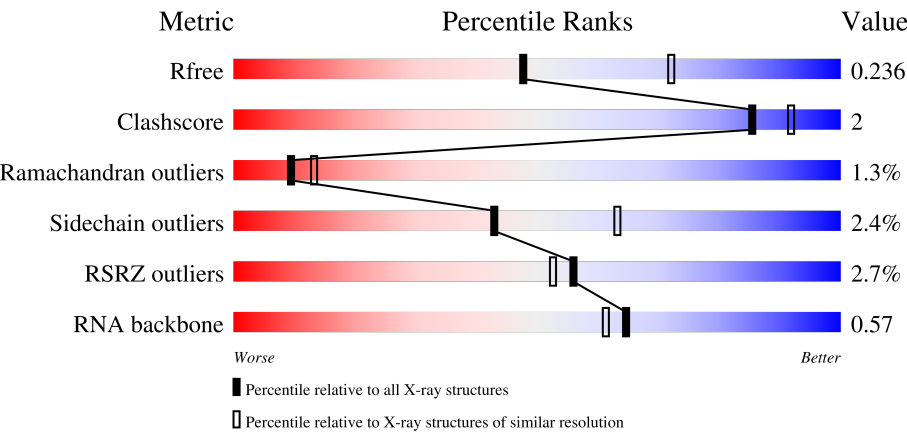
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)
RNA backbone	3983	1058 (2.70-2.14)

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	246	
1	B	246	
1	C	246	
1	D	246	

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Mol	Chain	Length	Quality of chain
2	E	28	75% 18% 7%
2	F	28	61% 39%
3	H	24	17% 25% 8% 67%
3	I	24	17% 12% 12% • 71%
3	J	24	8% 17% 8% • 71%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9340 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 SWI5-dependent HO expression protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	235	Total	C	N	O	S	0	0	0
			1903	1226	302	373	2			
1	C	240	Total	C	N	O	S	0	1	0
			1945	1253	312	378	2			
1	B	238	Total	C	N	O	S	0	0	0
			1924	1241	307	374	2			
1	A	225	Total	C	N	O	S	0	0	0
			1821	1179	290	350	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	expression tag	UNP B3LQW9
D	2	PRO	-	expression tag	UNP B3LQW9
D	3	LEU	-	expression tag	UNP B3LQW9
D	4	GLY	-	expression tag	UNP B3LQW9
D	5	SER	-	expression tag	UNP B3LQW9
D	14	SER	CYS	engineered mutation	UNP B3LQW9
D	68	SER	CYS	engineered mutation	UNP B3LQW9
D	106	SER	CYS	engineered mutation	UNP B3LQW9
D	180	SER	CYS	engineered mutation	UNP B3LQW9
C	1	GLY	-	expression tag	UNP B3LQW9
C	2	PRO	-	expression tag	UNP B3LQW9
C	3	LEU	-	expression tag	UNP B3LQW9
C	4	GLY	-	expression tag	UNP B3LQW9
C	5	SER	-	expression tag	UNP B3LQW9
C	14	SER	CYS	engineered mutation	UNP B3LQW9
C	68	SER	CYS	engineered mutation	UNP B3LQW9
C	106	SER	CYS	engineered mutation	UNP B3LQW9
C	180	SER	CYS	engineered mutation	UNP B3LQW9
B	1	GLY	-	expression tag	UNP B3LQW9
B	2	PRO	-	expression tag	UNP B3LQW9
B	3	LEU	-	expression tag	UNP B3LQW9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLY	-	expression tag	UNP B3LQW9
B	5	SER	-	expression tag	UNP B3LQW9
B	14	SER	CYS	engineered mutation	UNP B3LQW9
B	68	SER	CYS	engineered mutation	UNP B3LQW9
B	106	SER	CYS	engineered mutation	UNP B3LQW9
B	180	SER	CYS	engineered mutation	UNP B3LQW9
A	1	GLY	-	expression tag	UNP B3LQW9
A	2	PRO	-	expression tag	UNP B3LQW9
A	3	LEU	-	expression tag	UNP B3LQW9
A	4	GLY	-	expression tag	UNP B3LQW9
A	5	SER	-	expression tag	UNP B3LQW9
A	14	SER	CYS	engineered mutation	UNP B3LQW9
A	68	SER	CYS	engineered mutation	UNP B3LQW9
A	106	SER	CYS	engineered mutation	UNP B3LQW9
A	180	SER	CYS	engineered mutation	UNP B3LQW9

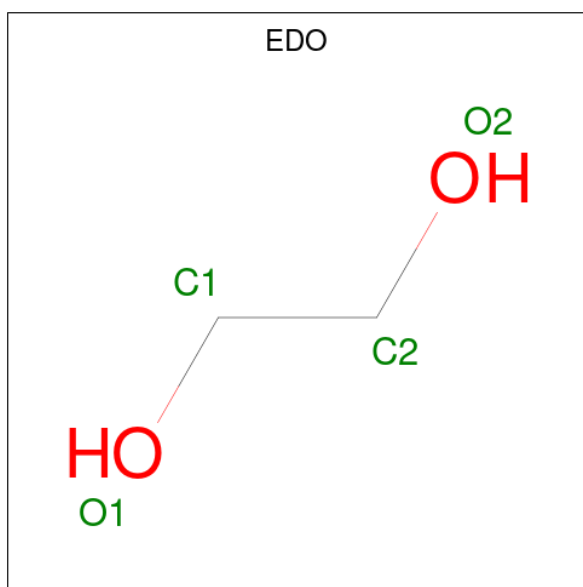
- Molecule 2 is a RNA chain called ASH1-E3 element, RNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	28	Total	C	N	O	P	0	0	0
			596	269	112	188	27			
2	F	28	Total	C	N	O	P	0	0	0
			596	269	112	188	27			

- Molecule 3 is a protein called SWI5-dependent HO expression protein 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	8	Total	C	N	O	0	0	0
			56	35	11	10			
3	J	7	Total	C	N	O	0	0	0
			46	31	7	8			
3	I	7	Total	C	N	O	0	0	0
			46	31	7	8			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

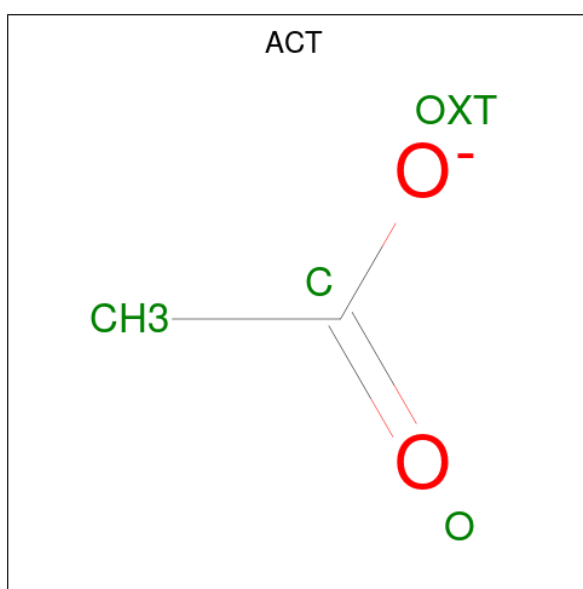
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	F	2	Total	Mg	0	0
			2	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

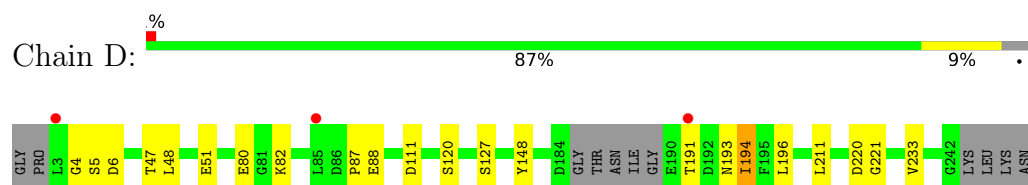
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	76	Total 76	O 76	0	0
7	C	69	Total 69	O 69	0	0
7	B	48	Total 48	O 48	0	0
7	A	45	Total 45	O 45	0	0
7	E	52	Total 52	O 52	0	0
7	F	39	Total 39	O 39	0	0
7	H	1	Total 1	O 1	0	0
7	J	3	Total 3	O 3	0	0

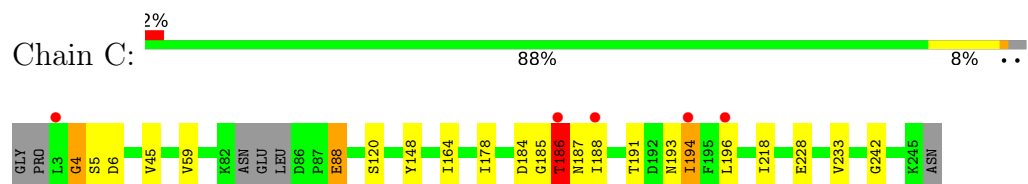
3 Residue-property plots [i](#)

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.

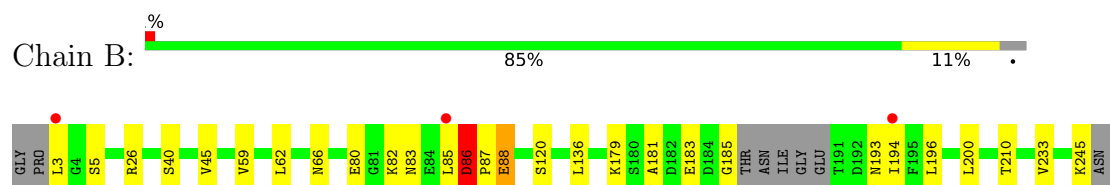
- Molecule 1: SWI5-dependent HO expression protein 2



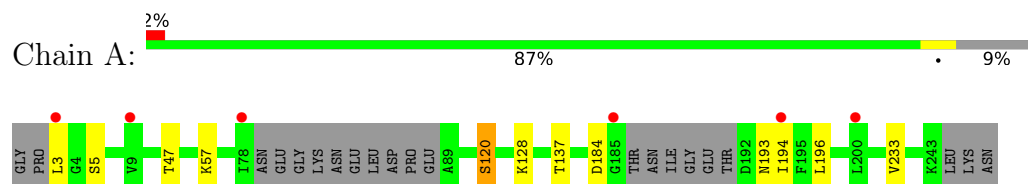
- Molecule 1: SWI5-dependent HO expression protein 2



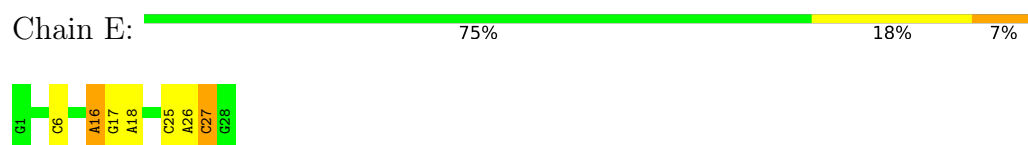
- Molecule 1: SWI5-dependent HO expression protein 2



- Molecule 1: SWI5-dependent HO expression protein 2



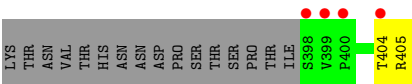
- Molecule 2: ASH1-E3 element, RNA (28-MER)



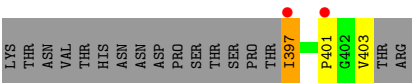
- Molecule 2: ASH1-E3 element, RNA (28-MER)



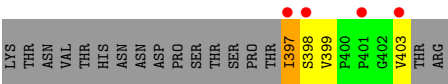
● Molecule 3: SWI5-dependent HO expression protein 3



● Molecule 3: SWI5-dependent HO expression protein 3



● Molecule 3: SWI5-dependent HO expression protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.52Å 58.34Å 146.01Å 90.00° 126.98° 90.00°	Depositor
Resolution (Å)	50.01 – 2.41 50.01 – 2.41	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.01-2.41) 90.4 (50.01-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.189 , 0.235 0.191 , 0.236	Depositor DCC
R_{free} test set	2571 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9340	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: MG, ACT, EDO

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	1.16	3/1854 (0.2%)	1.10	1/2507 (0.0%)
1	B	1.27	8/1959 (0.4%)	1.19	5/2650 (0.2%)
1	C	1.32	6/1981 (0.3%)	1.16	5/2680 (0.2%)
1	D	1.26	5/1938 (0.3%)	1.19	8/2624 (0.3%)
2	E	0.79	1/668 (0.1%)	1.24	7/1039 (0.7%)
2	F	0.81	1/668 (0.1%)	1.20	6/1039 (0.6%)
3	H	1.13	0/57	0.93	0/78
3	I	0.66	0/47	1.12	0/65
3	J	0.91	0/47	1.31	0/65
All	All	1.20	24/9219 (0.3%)	1.17	32/12747 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	ASP	N-CA	6.81	1.50	1.46
1	D	191	THR	CA-C	6.58	1.60	1.52
1	B	66	ASN	CA-C	6.45	1.61	1.52
1	C	4	GLY	N-CA	6.03	1.54	1.45
1	D	221	GLY	N-CA	5.98	1.54	1.45
1	A	128	LYS	C-O	-5.96	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	88	GLU	CA-C	5.95	1.60	1.52
1	C	45	VAL	C-O	-5.85	1.17	1.24
1	D	6	ASP	N-CA	5.85	1.53	1.46
1	B	59	VAL	N-CA	-5.68	1.39	1.46
1	B	88	GLU	CA-C	5.62	1.60	1.52
1	C	188	ILE	CA-CB	5.56	1.60	1.54
1	B	136	LEU	C-O	-5.50	1.16	1.23
1	D	127	SER	CA-C	5.49	1.59	1.52
2	F	26	A	O3'-P	-5.46	1.52	1.61
1	C	184	ASP	CA-C	5.41	1.59	1.52
1	B	62	LEU	CA-C	5.34	1.59	1.52
1	C	59	VAL	CA-C	5.31	1.59	1.52
1	A	120	SER	CB-OG	-5.24	1.31	1.42
1	C	88	GLU	CA-C	5.22	1.60	1.52
1	B	40	SER	CB-OG	5.17	1.52	1.42
1	B	45	VAL	C-O	-5.17	1.17	1.24
2	E	6	C	P-OP2	5.11	1.59	1.49
1	B	26	ARG	CA-C	5.00	1.59	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	GLY	N-CA-C	10.71	138.56	113.18
1	D	220	ASP	N-CA-C	-10.66	94.51	110.28
1	B	80	GLU	N-CA-C	9.25	124.11	113.01
2	E	27	C	C1'-C2'-O2'	-9.24	97.94	111.80
1	D	191	THR	N-CA-C	8.32	122.12	109.23
1	B	86	ASP	CA-C-N	8.30	130.21	119.84
1	B	86	ASP	C-N-CA	8.30	130.21	119.84
1	D	220	ASP	CA-C-N	-8.29	105.16	121.41
1	D	220	ASP	C-N-CA	-8.29	105.16	121.41
2	E	26	A	N9-C1'-C2'	7.84	125.76	114.00
2	E	27	C	C2'-C3'-O3'	-7.53	98.21	109.50
2	F	3	U	C3'-C2'-O2'	7.43	121.85	110.70
1	D	220	ASP	O-C-N	-7.03	114.31	122.89
2	E	25	C	C2'-C3'-O3'	-6.89	103.37	113.70
2	F	25	C	C2'-C3'-O3'	-6.83	103.46	113.70
2	E	16	A	C1'-C2'-O2'	6.82	118.63	108.40
2	F	16	A	C1'-C2'-O2'	6.48	118.12	108.40
1	D	80	GLU	N-CA-C	-6.25	102.28	110.53
1	D	4	GLY	N-CA-C	6.16	127.78	113.18
2	E	18	A	C1'-C2'-O2'	-6.14	99.19	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASP	CB-CA-C	-5.97	107.82	116.54
2	F	18	A	C1'-C2'-O2'	-5.91	99.53	108.40
1	C	178	ILE	N-CA-C	5.83	116.02	110.42
1	D	221	GLY	N-CA-C	-5.65	99.78	113.18
1	C	242	GLY	N-CA-C	5.44	118.81	112.50
2	F	1	G	C2'-C3'-O3'	-5.39	105.61	113.70
2	F	25	C	C3'-C2'-O2'	5.39	118.78	110.70
1	B	88	GLU	CA-C-N	5.28	128.34	120.90
1	B	88	GLU	C-N-CA	5.28	128.34	120.90
2	E	26	A	C2'-C3'-O3'	-5.20	101.71	109.50
1	C	164	ILE	CA-C-N	5.12	124.97	120.10
1	C	164	ILE	C-N-CA	5.12	124.97	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	86	ASP	Peptide
1	C	6	ASP	Peptide
1	D	87	PRO	Peptide

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	1821	0	1824	5	0
1	B	1924	0	1924	6	0
1	C	1945	0	1940	7	0
1	D	1903	0	1890	11	0
2	E	596	0	304	1	0
2	F	596	0	304	2	0
3	H	56	0	59	2	0
3	I	46	0	50	12	0
3	J	46	0	50	5	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	24	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	12	2	0
4	E	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
6	E	12	0	9	0	0
6	F	4	0	3	0	0
7	A	45	0	0	1	0
7	B	48	0	0	0	0
7	C	69	0	0	0	0
7	D	76	0	0	0	0
7	E	52	0	0	0	0
7	F	39	0	0	0	0
7	H	1	0	0	1	0
7	J	3	0	0	0	0
All	All	9340	0	8429	39	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 2.

All (39) 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:C:194:ILE:HG22	3:I:397:ILE:HB	1.58	0.84
1:D:194:ILE:HG22	3:J:397:ILE:HB	1.70	0.73
3:I:397:ILE:HG23	3:I:399:VAL:HG23	1.71	0.71
1:C:218:ILE:HD13	3:I:398:SER:O	1.92	0.70
1:C:194:ILE:CG2	3:I:397:ILE:HB	2.26	0.62
1:D:194:ILE:CG2	3:J:397:ILE:HB	2.31	0.60
1:C:185:GLY:O	1:C:186:THR:OG1	2.16	0.59
1:B:86:ASP:O	1:B:88:GLU:N	2.30	0.59
1:D:193:ASN:HB3	1:D:196:LEU:HD12	1.85	0.59
1:C:193:ASN:HB3	1:C:196:LEU:HD12	1.84	0.58
3:I:399:VAL:HG11	3:I:403:VAL:CG2	2.32	0.58
1:A:193:ASN:HB3	1:A:196:LEU:HD12	1.87	0.56
3:I:399:VAL:HG11	3:I:403:VAL:HG22	1.87	0.56
3:I:399:VAL:CG1	3:I:403:VAL:CG2	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:THR:HG21	1:A:47:THR:HG21	1.89	0.54
1:B:193:ASN:HB3	1:B:196:LEU:HD12	1.89	0.53
1:A:57:LYS:HE3	7:A:423:HOH:O	2.08	0.53
1:D:111:ASP:OD1	4:D:302:EDO:H21	2.08	0.53
1:D:194:ILE:HG22	3:J:397:ILE:CB	2.41	0.51
1:D:211:LEU:HD22	3:J:403:VAL:HG23	1.93	0.51
1:C:194:ILE:HG22	3:I:397:ILE:CB	2.37	0.50
1:B:181:ALA:O	1:B:185:GLY:N	2.40	0.49
3:I:399:VAL:CG1	3:I:403:VAL:HG22	2.44	0.48
3:I:397:ILE:HG23	3:I:397:ILE:O	2.14	0.48
2:E:16:A:C5	2:E:17:G:H1'	2.50	0.46
1:A:137:THR:HG23	1:A:233:VAL:HG12	1.98	0.46
1:D:194:ILE:HG22	3:J:397:ILE:CG2	2.47	0.45
3:H:404:THR:HG22	7:H:501:HOH:O	2.18	0.44
1:B:83:ASN:C	1:B:85:LEU:H	2.26	0.44
3:I:399:VAL:HG11	3:I:403:VAL:HG21	2.00	0.43
1:B:200:LEU:HD21	3:H:405:ARG:HD3	2.01	0.43
1:C:148:TYR:CD2	4:C:305:EDO:H22	2.54	0.42
3:I:399:VAL:CG1	3:I:403:VAL:HG21	2.48	0.42
1:D:48:LEU:HA	1:D:51:GLU:OE1	2.19	0.42
1:D:148:TYR:CD2	4:D:302:EDO:H12	2.55	0.41
2:F:8:G:C8	2:F:8:G:H3'	2.54	0.41
1:D:47:THR:HG21	1:A:47:THR:CG2	2.50	0.41
2:F:4:A:C2	2:F:23:A:C2	3.08	0.41
1:B:179:LYS:O	1:B:183:GLU:HG3	2.22	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	219/246 (89%)	211 (96%)	7 (3%)	1 (0%)	24 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	234/246 (95%)	223 (95%)	8 (3%)	3 (1%)	9	13
1	C	237/246 (96%)	225 (95%)	7 (3%)	5 (2%)	5	6
1	D	231/246 (94%)	224 (97%)	5 (2%)	2 (1%)	14	20
3	H	6/24 (25%)	6 (100%)	0	0	100	100
3	I	5/24 (21%)	4 (80%)	1 (20%)	0	100	100
3	J	5/24 (21%)	4 (80%)	0	1 (20%)	0	0
All	All	937/1056 (89%)	897 (96%)	28 (3%)	12 (1%)	9	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	194	ILE
1	C	194	ILE
1	B	86	ASP
1	B	87	PRO
1	A	194	ILE
1	C	4	GLY
1	C	186	THR
1	C	191	THR
3	J	401	PRO
1	C	88	GLU
1	D	82	LYS
1	B	194	ILE

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	206/224 (92%)	203 (98%)	3 (2%)	57	75
1	B	218/224 (97%)	211 (97%)	7 (3%)	34	54
1	C	220/224 (98%)	214 (97%)	6 (3%)	39	60
1	D	216/224 (96%)	213 (99%)	3 (1%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	7/23 (30%)	7 (100%)	0	100	100
3	I	6/23 (26%)	5 (83%)	1 (17%)	2	2
3	J	6/23 (26%)	5 (83%)	1 (17%)	2	2
All	All	879/965 (91%)	858 (98%)	21 (2%)	43	63

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	5	SER
1	D	120	SER
1	D	233	VAL
1	C	5	SER
1	C	120	SER
1	C	186	THR
1	C	187	ASN
1	C	228	GLU
1	C	233	VAL
1	B	3	LEU
1	B	5	SER
1	B	82	LYS
1	B	120	SER
1	B	210	THR
1	B	233	VAL
1	B	245	LYS
1	A	3	LEU
1	A	5	SER
1	A	120	SER
3	J	397	ILE
3	I	397	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	19	GLN
1	D	41	HIS
1	D	203	ASN
1	C	167	ASN
1	B	41	HIS
1	A	19	GLN
1	A	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	27/28 (96%)	1 (3%)	0
2	F	27/28 (96%)	2 (7%)	0
All	All	54/56 (96%)	3 (5%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	27	C
2	F	17	G
2	F	28	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\# Z > 2$
6	ACT	D	304	-	3,3,3	0.91	0	3,3,3	0.61	0
6	ACT	B	303	-	3,3,3	0.94	0	3,3,3	0.92	0
6	ACT	E	103	-	3,3,3	0.96	0	3,3,3	0.70	0
6	ACT	E	104	-	3,3,3	0.98	0	3,3,3	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	F	103	-	3,3,3	1.26	0	3,3,3	0.44	0
4	EDO	E	101	-	3,3,3	0.68	0	2,2,2	0.21	0
4	EDO	C	302	-	3,3,3	0.64	0	2,2,2	0.21	0
4	EDO	C	304	-	3,3,3	0.69	0	2,2,2	0.24	0
4	EDO	C	305	-	3,3,3	0.51	0	2,2,2	0.17	0
4	EDO	B	301	-	3,3,3	0.64	0	2,2,2	0.41	0
4	EDO	C	306	-	3,3,3	0.75	0	2,2,2	0.84	0
4	EDO	A	301	-	3,3,3	0.58	0	2,2,2	0.19	0
4	EDO	D	302	-	3,3,3	0.67	0	2,2,2	0.59	0
4	EDO	C	301	-	3,3,3	0.41	0	2,2,2	0.57	0
4	EDO	D	301	-	3,3,3	0.30	0	2,2,2	0.56	0
6	ACT	E	102	-	3,3,3	0.65	0	3,3,3	1.23	0
4	EDO	C	303	-	3,3,3	0.59	0	2,2,2	0.36	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
4	EDO	E	101	-	-	1/1/1/1	-
4	EDO	C	302	-	-	1/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-
4	EDO	C	305	-	-	0/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	D	302	-	-	0/1/1/1	-
4	EDO	C	301	-	-	1/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-
4	EDO	C	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	306	EDO	O1-C1-C2-O2
4	B	301	EDO	O1-C1-C2-O2
4	A	301	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	302	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2
4	C	303	EDO	O1-C1-C2-O2
4	E	101	EDO	O1-C1-C2-O2
4	C	301	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	305	EDO	1	0
4	D	302	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	225/246 (91%)	0.18	6 (2%)	56	52	35, 67, 115, 131	1 (0%)
1	B	238/246 (96%)	0.00	3 (1%)	75	72	33, 63, 118, 153	1 (0%)
1	C	240/246 (97%)	-0.24	5 (2%)	63	60	19, 49, 103, 137	1 (0%)
1	D	235/246 (95%)	-0.23	3 (1%)	75	72	32, 50, 113, 156	0
2	E	28/28 (100%)	-0.88	0	100	100	41, 52, 75, 84	0
2	F	28/28 (100%)	-0.62	0	100	100	40, 57, 95, 101	0
3	H	8/24 (33%)	2.06	4 (50%)	0	0	100, 115, 121, 145	0
3	I	7/24 (29%)	2.45	4 (57%)	0	0	98, 112, 123, 139	0
3	J	7/24 (29%)	1.88	2 (28%)	1	1	48, 92, 96, 105	1 (14%)
All	All	1016/1112 (91%)	-0.07	27 (2%)	56	52	19, 58, 116, 156	4 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	LEU	5.4
1	A	185	GLY	4.5
3	J	401	PRO	4.2
3	I	397	ILE	4.0
1	B	3	LEU	4.0
3	H	398	SER	3.9
1	C	3	LEU	3.8
1	C	188	ILE	3.7
3	I	398	SER	3.6
3	I	401	PRO	3.5
1	A	9	VAL	3.3
1	A	3	LEU	3.2
1	B	194	ILE	3.2
1	A	194	ILE	3.0
3	H	399	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	186	THR	2.8
1	A	78	ILE	2.8
3	H	404	THR	2.7
3	I	403	VAL	2.6
3	J	397	ILE	2.5
1	C	194	ILE	2.5
1	A	200	LEU	2.3
1	D	85	LEU	2.3
1	C	196	LEU	2.2
1	D	191	THR	2.1
1	B	85	LEU	2.1
3	H	400	PRO	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(Å ²)	Q<0.9
6	ACT	F	103	4/4	0.66	0.21	51,53,55,66	0
6	ACT	E	102	4/4	0.74	0.24	69,70,70,77	0
4	EDO	C	302	4/4	0.76	0.20	66,68,75,77	0
6	ACT	E	103	4/4	0.79	0.23	66,67,71,76	0
6	ACT	E	104	4/4	0.79	0.20	55,60,66,70	0
4	EDO	E	101	4/4	0.79	0.15	66,70,78,79	0
6	ACT	B	303	4/4	0.82	0.16	53,58,58,60	0
6	ACT	D	304	4/4	0.86	0.20	63,77,77,82	0
4	EDO	A	301	4/4	0.86	0.21	68,83,88,91	0
4	EDO	C	306	4/4	0.87	0.18	59,70,74,77	0
5	MG	B	302	1/1	0.89	0.29	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	F	102	1/1	0.89	0.09	49,49,49,49	0
4	EDO	C	305	4/4	0.91	0.12	46,50,51,53	0
5	MG	F	101	1/1	0.91	0.09	57,57,57,57	0
4	EDO	C	301	4/4	0.91	0.13	57,58,58,60	0
5	MG	A	302	1/1	0.92	0.21	71,71,71,71	0
4	EDO	D	302	4/4	0.93	0.11	44,44,45,50	0
4	EDO	C	303	4/4	0.93	0.15	55,56,57,67	0
4	EDO	B	301	4/4	0.94	0.10	56,57,65,65	0
5	MG	D	303	1/1	0.94	0.19	60,60,60,60	0
4	EDO	C	304	4/4	0.94	0.12	53,55,55,59	0
4	EDO	D	301	4/4	0.95	0.10	59,62,63,65	0
5	MG	C	307	1/1	0.95	0.22	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.