Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2024 – 12:10 pm GMT

PDB ID	:	5M0I
Title	:	Crystal structure of the nuclear complex with She2p and the ASH1 mRNA E3-localization element
Authors	:	Edelmann, 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 (i) 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 (i)) were used in the production of this report:

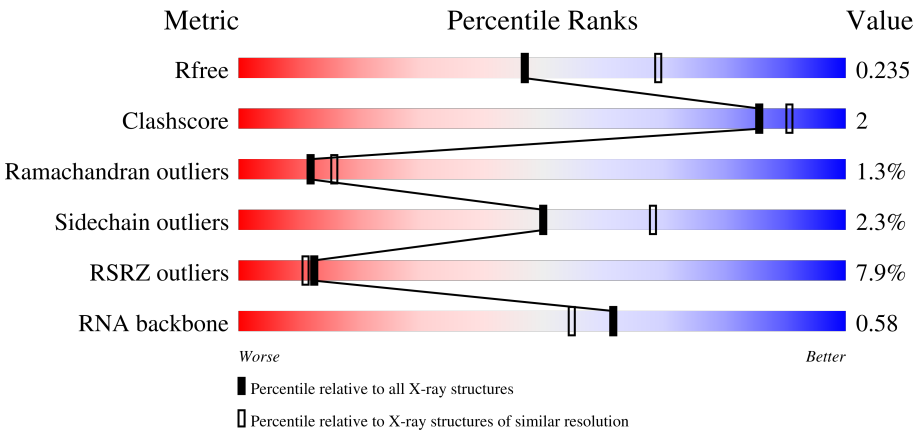
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)
RNA backbone	3102	1080 (2.80-2.04)

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 <=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	9% 85% 5% • 9%
1	B	246	5% 87% 9% •
1	C	246	4% 90% 7% • •
1	D	246	9% 87% 7% • •

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Mol	Chain	Length	Quality of chain
2	E	28	61% 32% 7%
2	F	28	7% 71% 29%
3	H	24	12% 25% 8% 67%
3	I	24	29% 12% 17% 71%
3	J	24	12% 17% 12% 71%

2 Entry composition (i)

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

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

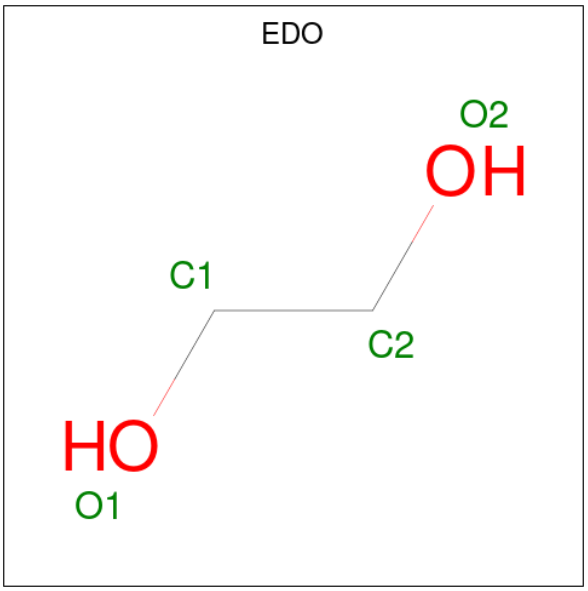
- Molecule 2 is a RNA chain called ASH1-E3 element, RNA (28-MER).

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

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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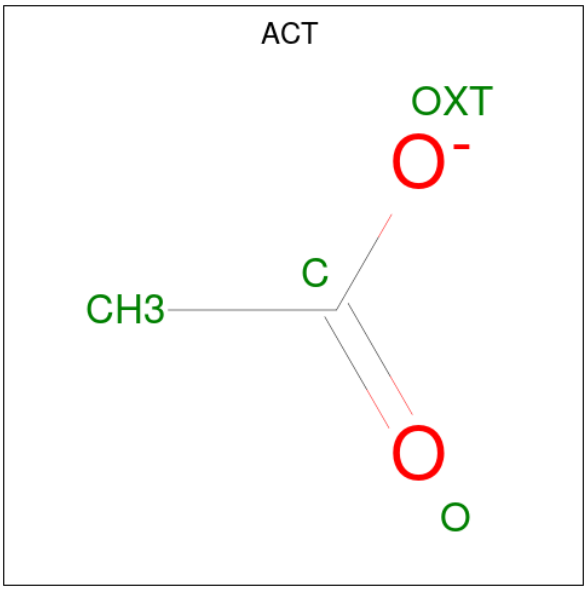
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	F	2	Total Mg 2 2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

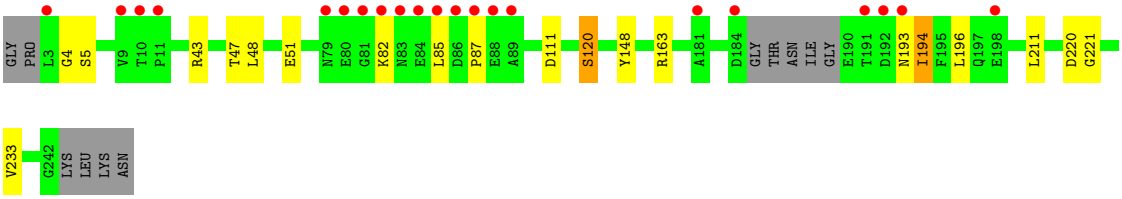
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	D	76	76	76	0	0
			Total	O		
7	C	69	69	69	0	0
			Total	O		
7	B	48	48	48	0	0
			Total	O		
7	A	45	45	45	0	0
			Total	O		
7	E	52	52	52	0	0
			Total	O		
7	F	39	39	39	0	0
			Total	O		
7	H	1	1	1	0	0
			Total	O		
7	J	3	3	3	0	0

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.

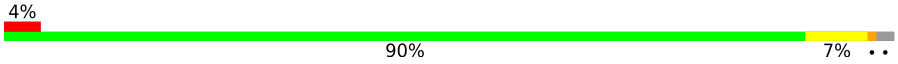
• Molecule 1: SWI5-dependent HO expression protein 2

Chain D:



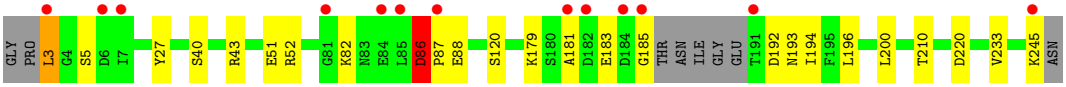
• Molecule 1: SWI5-dependent HO expression protein 2

Chain C:



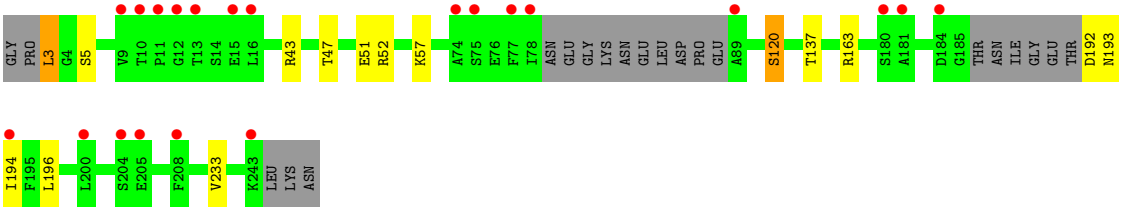
• Molecule 1: SWI5-dependent HO expression protein 2

Chain B:



• Molecule 1: SWI5-dependent HO expression protein 2

Chain A:



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

Chain E:

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

Chain F:

• Molecule 3: SWI5-dependent HO expression protein 3

Chain H:

• Molecule 3: SWI5-dependent HO expression protein 3

Chain J:

• Molecule 3: SWI5-dependent HO expression protein 3

Chain I:

4 Data and refinement statistics (i)

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 46.72 – 2.41	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.01-2.41) 90.4 (46.72-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.189 , 0.235 0.190 , 0.235	Depositor DCC
R_{free} test set	2571 reflections (4.92%)	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)	0.31 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.87	2/1854 (0.1%)	0.91	6/2507 (0.2%)
1	B	0.96	2/1959 (0.1%)	0.95	6/2650 (0.2%)
1	C	1.02	3/1981 (0.2%)	0.97	4/2680 (0.1%)
1	D	0.95	2/1938 (0.1%)	0.95	10/2624 (0.4%)
2	E	0.95	1/668 (0.1%)	1.21	12/1039 (1.2%)
2	F	0.99	2/668 (0.3%)	1.17	4/1039 (0.4%)
3	H	0.70	0/57	0.74	0/78
3	I	0.48	0/47	0.66	0/65
3	J	0.64	0/47	0.90	0/65
All	All	0.95	12/9219 (0.1%)	0.99	42/12747 (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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	SER	CB-OG	-8.13	1.31	1.42
1	B	40	SER	CB-OG	7.88	1.52	1.42
1	B	51	GLU	CD-OE1	7.03	1.33	1.25
2	F	26	A	O3'-P	-6.82	1.52	1.61
2	F	5	A	O3'-P	-6.10	1.53	1.61
2	E	6	C	P-OP2	6.01	1.59	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	GLU	CD-OE1	5.86	1.32	1.25
1	D	120	SER	CB-OG	-5.70	1.34	1.42
1	C	4	GLY	N-CA	5.38	1.54	1.46
1	D	221	GLY	N-CA	5.33	1.54	1.46
1	C	50	PHE	CG-CD1	5.21	1.46	1.38
1	C	115	TYR	CE1-CZ	5.03	1.45	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	27	C	O5'-P-OP1	-11.66	95.20	105.70
1	B	220	ASP	CB-CG-OD1	10.37	127.63	118.30
2	F	27	C	O5'-P-OP2	10.23	122.98	110.70
1	B	220	ASP	CB-CG-OD2	-10.21	109.11	118.30
1	C	4	GLY	N-CA-C	10.19	138.56	113.10
2	E	26	A	N9-C1'-C2'	9.05	125.76	114.00
1	D	220	ASP	C-N-CA	-8.16	105.16	122.30
2	E	14	A	O5'-P-OP2	-7.70	98.77	105.70
2	E	22	U	O5'-P-OP1	-7.17	99.25	105.70
1	A	43	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	C	163	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	E	17	G	O5'-P-OP2	6.94	119.03	110.70
1	A	163	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	163	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	163	ARG	NE-CZ-NH1	6.79	123.70	120.30
2	F	27	C	N3-C4-C5	-6.59	119.26	121.90
1	A	52	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	E	26	A	O5'-P-OP2	-6.48	99.87	105.70
1	C	163	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	43	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	220	ASP	N-CA-C	-6.11	94.51	111.00
2	E	4	A	O5'-P-OP1	-6.05	100.25	105.70
1	B	43	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	4	GLY	N-CA-C	5.87	127.78	113.10
2	E	26	A	O4'-C1'-N9	5.77	112.81	108.20
2	E	19	C	O5'-P-OP2	-5.76	100.51	105.70
1	B	52	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	E	26	A	C3'-C2'-C1'	-5.53	97.08	101.50
1	D	220	ASP	CA-C-N	5.52	127.24	116.20
2	F	26	A	O5'-P-OP2	-5.50	100.75	105.70
2	E	12	C	O5'-P-OP2	5.44	117.23	110.70
1	D	85	LEU	CA-CB-CG	5.37	127.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	221	GLY	N-CA-C	-5.33	99.78	113.10
1	D	220	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	D	220	ASP	O-C-N	-5.23	114.31	123.20
1	B	3	LEU	CB-CG-CD2	5.22	119.88	111.00
1	A	3	LEU	CB-CG-CD2	5.22	119.88	111.00
2	E	15	A	O5'-P-OP2	-5.16	101.06	105.70
1	D	43	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	43	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	E	27	C	C2'-C3'-O3'	-5.13	98.21	109.50
1	B	27	TYR	CB-CG-CD1	5.05	124.03	121.00

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	5	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
4	D	8	0	12	2	0
4	E	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	38	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 (38) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	219/246 (89%)	211 (96%)	7 (3%)	1 (0%)	29 40
1	B	234/246 (95%)	223 (95%)	8 (3%)	3 (1%)	12 16
1	C	237/246 (96%)	225 (95%)	7 (3%)	5 (2%)	7 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	231/246 (94%)	224 (97%)	5 (2%)	2 (1%)	17	24
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%)	12	16

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 (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	206/224 (92%)	202 (98%)	4 (2%)	57	74
1	B	218/224 (97%)	210 (96%)	8 (4%)	34	51
1	C	220/224 (98%)	215 (98%)	5 (2%)	50	68
1	D	216/224 (96%)	213 (99%)	3 (1%)	67	81
3	H	7/23 (30%)	7 (100%)	0	100	100
3	I	6/23 (26%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	6/23 (26%)	6 (100%)	0	100	100
All	All	879/965 (91%)	859 (98%)	20 (2%)	50	68

All (20) 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	233	VAL
1	B	3	LEU
1	B	5	SER
1	B	82	LYS
1	B	120	SER
1	B	192	ASP
1	B	210	THR
1	B	233	VAL
1	B	245	LYS
1	A	3	LEU
1	A	5	SER
1	A	120	SER
1	A	192	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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 (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 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	$\#\|Z\| > 2$
4	EDO	D	301	-	3,3,3	0.32	0	2,2,2	0.52	0
4	EDO	C	303	-	3,3,3	0.61	0	2,2,2	0.36	0
6	ACT	B	303	-	3,3,3	0.88	0	3,3,3	0.92	0
6	ACT	D	304	-	3,3,3	0.85	0	3,3,3	0.60	0
6	ACT	E	104	-	3,3,3	0.92	0	3,3,3	0.77	0
4	EDO	D	302	-	3,3,3	0.68	0	2,2,2	0.68	0
4	EDO	C	302	-	3,3,3	0.68	0	2,2,2	0.16	0
4	EDO	C	301	-	3,3,3	0.45	0	2,2,2	0.54	0
4	EDO	C	306	-	3,3,3	0.78	0	2,2,2	0.95	0
6	ACT	E	102	-	3,3,3	0.61	0	3,3,3	1.24	0
4	EDO	C	304	-	3,3,3	0.72	0	2,2,2	0.32	0
4	EDO	B	301	-	3,3,3	0.65	0	2,2,2	0.45	0
4	EDO	C	305	-	3,3,3	0.53	0	2,2,2	0.14	0
4	EDO	A	301	-	3,3,3	0.60	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ACT	E	103	-	3,3,3	0.91	0	3,3,3	0.69	0
4	EDO	E	101	-	3,3,3	0.71	0	2,2,2	0.16	0
6	ACT	F	103	-	3,3,3	1.19	0	3,3,3	0.43	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	D	301	-	-	1/1/1/1	-
4	EDO	C	303	-	-	1/1/1/1	-
4	EDO	D	302	-	-	0/1/1/1	-
4	EDO	C	302	-	-	1/1/1/1	-
4	EDO	C	301	-	-	1/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	C	305	-	-	0/1/1/1	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	E	101	-	-	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
4	C	302	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
4	C	303	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2
4	C	301	EDO	O1-C1-C2-O2
4	E	101	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	D	302	EDO	2	0
4	C	305	EDO	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.30	21 (9%)	8	7	35, 68, 115, 131	1 (0%)
1	B	238/246 (96%)	0.08	13 (5%)	25	23	33, 63, 118, 153	1 (0%)
1	C	240/246 (97%)	0.10	10 (4%)	36	34	31, 49, 103, 137	0
1	D	235/246 (95%)	0.25	21 (8%)	9	8	32, 50, 113, 156	0
2	E	28/28 (100%)	-0.70	0	100	100	41, 52, 75, 84	0
2	F	28/28 (100%)	-0.18	2 (7%)	16	14	40, 57, 95, 101	0
3	H	8/24 (33%)	1.66	3 (37%)	0	0	100, 115, 121, 145	0
3	I	7/24 (29%)	4.61	7 (100%)	0	0	98, 112, 123, 139	0
3	J	7/24 (29%)	2.36	3 (42%)	0	0	88, 94, 96, 105	1 (14%)
All	All	1016/1112 (91%)	0.20	80 (7%)	12	11	31, 58, 116, 156	3 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	397	ILE	7.2
3	J	401	PRO	6.3
3	I	401	PRO	6.2
1	A	11	PRO	5.8
1	D	83	ASN	5.8
1	A	78	ILE	5.7
1	B	185	GLY	5.6
3	I	398	SER	5.5
1	D	85	LEU	5.4
1	D	82	LYS	5.3
1	D	80	GLU	5.1
1	B	3	LEU	5.0
1	D	81	GLY	4.9
1	B	191	THR	4.9
1	D	87	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	243	LYS	4.7
1	A	75	SER	4.7
1	D	191	THR	4.4
3	I	399	VAL	4.3
1	C	3	LEU	4.2
1	C	191	THR	4.2
1	D	192	ASP	4.1
1	D	84	GLU	4.1
1	B	6	ASP	4.1
1	C	244	LEU	4.1
3	J	397	ILE	4.0
1	A	9	VAL	4.0
1	B	7	ILE	3.9
1	D	88	GLU	3.8
3	I	400	PRO	3.6
1	C	245	LYS	3.3
3	I	403	VAL	3.3
1	C	192	ASP	3.2
1	C	190	GLU	3.2
1	D	89	ALA	3.1
1	B	85	LEU	3.1
1	B	181	ALA	3.0
1	C	188	ILE	3.0
1	A	77	PHE	2.9
3	J	400	PRO	2.9
3	H	402	GLY	2.9
2	F	16	A	2.9
1	A	184	ASP	2.9
1	D	184	ASP	2.8
1	D	193	ASN	2.8
1	D	11	PRO	2.7
3	H	400	PRO	2.7
1	B	245	LYS	2.6
3	H	405	ARG	2.6
1	A	89	ALA	2.6
1	C	185	GLY	2.6
1	A	205	GLU	2.6
1	D	3	LEU	2.5
1	D	181	ALA	2.5
1	B	184	ASP	2.5
1	A	12	GLY	2.5
1	A	15	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	180	SER	2.4
1	B	182	ASP	2.4
1	A	74	ALA	2.4
1	A	200	LEU	2.4
1	B	81	GLY	2.3
1	D	10	THR	2.3
1	D	86	ASP	2.3
3	I	402	GLY	2.2
1	A	10	THR	2.2
1	A	16	LEU	2.2
1	D	79	ASN	2.2
1	C	198	GLU	2.2
1	A	181	ALA	2.2
1	C	186	THR	2.2
1	A	208	PHE	2.2
2	F	14	A	2.2
1	B	84	GLU	2.2
1	A	204	SER	2.2
1	B	87	PRO	2.1
1	A	194	ILE	2.1
1	D	198	GLU	2.1
1	D	9	VAL	2.0
1	A	13	THR	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	301	4/4	0.74	0.29	68,83,88,91	0
4	EDO	E	101	4/4	0.81	0.20	66,70,78,79	0
5	MG	A	302	1/1	0.84	0.53	71,71,71,71	0
4	EDO	C	302	4/4	0.86	0.18	66,68,75,77	0
5	MG	D	303	1/1	0.87	0.44	60,60,60,60	0
4	EDO	C	306	4/4	0.88	0.30	59,70,74,77	0
6	ACT	E	102	4/4	0.88	0.15	69,70,70,77	0
6	ACT	B	303	4/4	0.89	0.16	53,58,58,60	0
6	ACT	D	304	4/4	0.89	0.28	63,77,77,82	0
6	ACT	E	104	4/4	0.89	0.15	55,60,66,70	0
6	ACT	F	103	4/4	0.89	0.12	51,53,55,66	0
6	ACT	E	103	4/4	0.91	0.15	66,67,71,76	0
5	MG	F	102	1/1	0.91	0.18	49,49,49,49	0
4	EDO	C	304	4/4	0.91	0.15	53,55,55,59	0
5	MG	F	101	1/1	0.92	0.08	57,57,57,57	0
4	EDO	C	303	4/4	0.92	0.22	55,56,57,67	0
4	EDO	D	302	4/4	0.93	0.19	44,44,45,50	0
4	EDO	C	305	4/4	0.94	0.22	46,50,51,53	0
4	EDO	D	301	4/4	0.94	0.22	59,62,63,65	0
4	EDO	B	301	4/4	0.95	0.25	56,57,65,65	0
5	MG	B	302	1/1	0.96	0.78	80,80,80,80	0
4	EDO	C	301	4/4	0.97	0.17	57,58,58,60	0
5	MG	C	307	1/1	0.97	0.68	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.