



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:51 PM UTC

PDB ID : 4FVA / pdb_00004fva
Title : Crystal structure of truncated *Caenorhabditis elegans* TDP2
Authors : Shi, K.; Kurahashi, K.; Aihara, H.
Deposited on : 2012-06-29
Resolution : 2.07 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

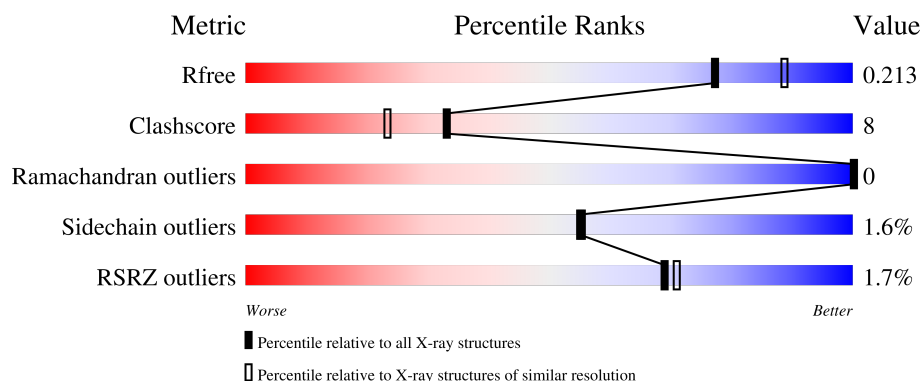
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. 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	256	2% 84% 13% ..
1	B	256	% 86% 11% ..
1	C	256	3% 81% 15% ..
1	D	256	% 85% 11% ..

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
2	EDO	B	405	-	-	X	-

2 Entry composition [i](#)

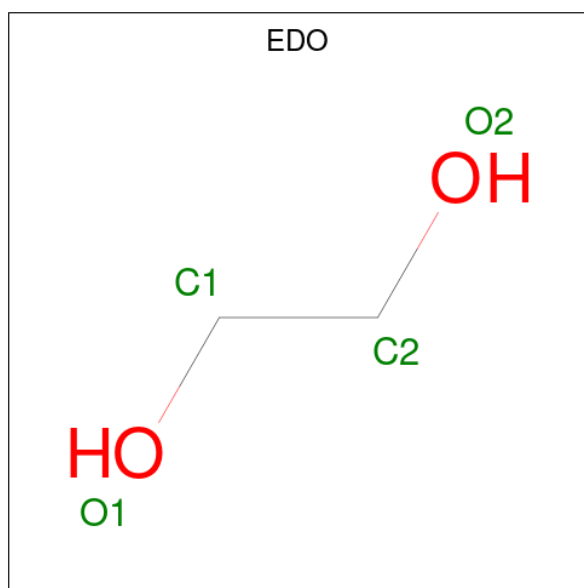
There are 5 unique types of molecules in this entry. The entry contains 8850 atoms, of which 112 are hydrogens and 0 are deuteriums.

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 5'-tyrosyl-DNA phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			2013	1285	353	364	11			
1	B	250	Total	C	N	O	S	0	0	0
			2022	1290	354	367	11			
1	C	251	Total	C	N	O	S	0	0	0
			2027	1293	355	368	11			
1	D	248	Total	C	N	O	S	0	0	0
			2001	1275	350	365	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

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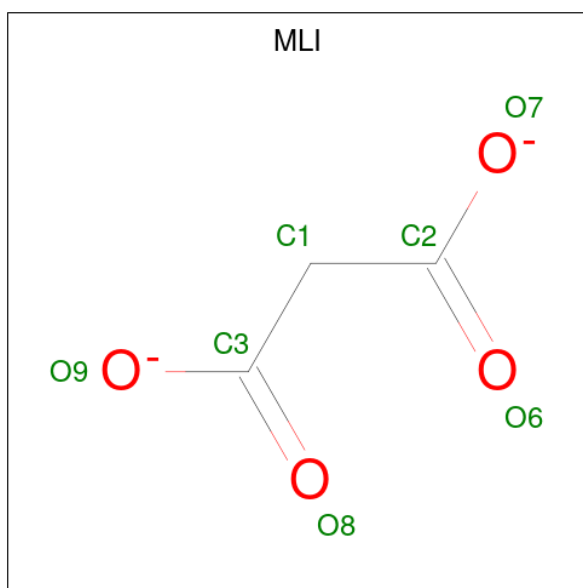
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $\text{C}_3\text{H}_2\text{O}_4$).

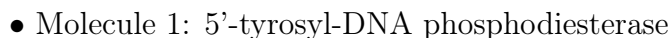
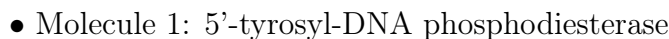
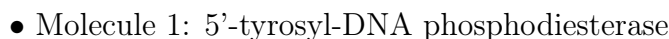


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			9	3	2	4		
4	B	1	Total	C	H	O	0	0
			9	3	2	4		
4	B	1	Total	C	H	O	0	0
			9	3	2	4		
4	C	1	Total	C	H	O	0	0
			9	3	2	4		
4	D	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	2
			141	141		
5	B	149	Total	O	0	1
			150	150		
5	C	149	Total	O	0	1
			150	150		
5	D	127	Total	O	0	0
			127	127		

- Molecule 1: 5'-tyrosyl-DNA phosphodiesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.60Å 104.40Å 84.70Å 90.00° 90.98° 90.00°	Depositor
Resolution (Å)	44.99 – 2.07 44.99 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.99-2.07) 99.2 (44.99-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1066)	Depositor
R, R_{free}	0.159 , 0.211 0.165 , 0.213	Depositor DCC
R_{free} test set	1991 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8850	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2622e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, MG, 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	0.46	0/2060	0.83	4/2777 (0.1%)
1	B	0.47	0/2069	0.81	5/2789 (0.2%)
1	C	0.45	0/2074	0.83	7/2796 (0.3%)
1	D	0.44	0/2045	0.80	0/2755
All	All	0.46	0/8248	0.81	16/11117 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	PHE	N-CA-C	-7.12	100.26	110.59
1	C	282	VAL	CA-C-N	6.53	126.51	119.78
1	C	282	VAL	C-N-CA	6.53	126.51	119.78
1	A	280	SER	CA-C-O	6.46	121.69	117.94
1	C	280	SER	CA-C-O	6.11	121.48	117.94
1	A	280	SER	CB-CA-C	-6.08	108.32	117.07
1	C	113	GLU	N-CA-C	-5.94	105.86	114.12
1	B	328	GLY	CA-C-N	5.92	127.24	119.84
1	B	328	GLY	C-N-CA	5.92	127.24	119.84
1	B	280	SER	CA-C-O	5.55	121.16	117.94
1	C	280	SER	CB-CA-C	-5.43	109.24	117.07
1	A	280	SER	N-CA-C	5.31	113.13	108.78
1	B	280	SER	CB-CA-C	-5.22	109.55	117.07
1	C	165	ALA	CA-C-N	-5.16	113.61	119.28
1	C	165	ALA	C-N-CA	-5.16	113.61	119.28
1	B	149	VAL	N-CA-C	-5.01	105.66	110.72

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	2013	0	1982	32	0
1	B	2022	0	1988	29	0
1	C	2027	0	1993	39	0
1	D	2001	0	1971	25	0
2	A	16	24	24	2	0
2	B	24	36	36	6	0
2	C	16	24	24	0	0
2	D	12	18	18	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	7	2	2	0	0
4	B	14	4	4	1	0
4	C	7	2	2	1	0
4	D	7	2	2	0	0
5	A	141	0	0	4	0
5	B	150	0	0	4	0
5	C	150	0	0	6	0
5	D	127	0	0	2	0
All	All	8738	112	8046	126	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 (126) 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:311:LYS:HE3	5:C:647:HOH:O	1.42	1.19
1:B:113:GLU:HG2	1:B:114:ASP:N	1.66	1.06
1:B:113:GLU:HG2	1:B:114:ASP:H	0.88	1.03
1:B:113:GLU:CG	1:B:114:ASP:H	1.73	1.01
1:C:210:MET:HE1	1:C:235:SER:H	1.26	1.00
1:A:284:ASP:HA	5:A:573:HOH:O	1.64	0.96
1:C:210:MET:CE	1:C:234:GLU:HG3	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:GLU:N	1:D:116:LYS:HG2	1.86	0.91
1:C:180:ASN:ND2	1:C:183:CYS:SG	2.55	0.80
1:B:131:ASP:HB2	5:B:639:HOH:O	1.82	0.79
1:D:255:ARG:HH22	1:D:281:ARG:HG3	1.48	0.79
1:B:328:GLY:H	2:B:405:EDO:H21	1.51	0.76
1:A:275:ARG:HH12	2:A:405:EDO:H12	1.52	0.75
1:D:113:GLU:HG2	1:D:115:LEU:H	1.52	0.73
1:C:210:MET:HE1	1:C:235:SER:N	2.02	0.73
1:A:285:GLY:N	5:A:573:HOH:O	2.21	0.70
1:B:277:GLU:OE1	1:B:277:GLU:N	2.19	0.70
1:A:275:ARG:HB2	1:A:277:GLU:OE2	1.91	0.69
1:A:332:LYS:HE2	1:A:362:ALA:O	1.93	0.69
1:A:277:GLU:OE1	1:A:277:GLU:N	2.20	0.68
1:A:131:ASP:HB2	5:A:637:HOH:O	1.94	0.67
1:D:128:ASP:OD2	1:D:311:LYS:NZ	2.24	0.67
1:C:275:ARG:HG2	1:C:278:GLU:CD	2.21	0.66
1:C:112:ALA:N	5:C:648:HOH:O	2.28	0.66
1:D:275:ARG:HG2	1:D:278:GLU:CD	2.21	0.65
1:A:115:LEU:CD1	1:A:329:PRO:HB2	2.27	0.65
1:C:210:MET:HE2	1:C:234:GLU:HG3	1.77	0.65
1:A:253:LYS:NZ	1:A:257:ILE:HD11	2.13	0.64
1:C:318:LYS:O	1:C:319:MET:HE3	1.98	0.64
1:A:306:PHE:CE2	1:A:316:GLY:C	2.76	0.63
1:C:210:MET:CE	1:C:235:SER:H	2.06	0.62
2:B:407:EDO:H21	5:B:601:HOH:O	1.99	0.62
1:A:306:PHE:CE2	1:A:318:LYS:HG3	2.34	0.61
1:C:210:MET:HE3	1:C:234:GLU:HG3	1.80	0.61
1:A:115:LEU:HD12	1:A:329:PRO:HB2	1.83	0.60
1:C:319:MET:CE	1:C:319:MET:HA	2.31	0.60
1:C:125:TRP:CD2	1:C:355:ALA:HB2	2.36	0.59
1:C:253:LYS:NZ	5:C:639[B]:HOH:O	2.34	0.59
1:B:252:ASP:OD1	1:B:255:ARG:NH2	2.36	0.58
1:A:239:HIS:HD2	1:A:242:GLN:NE2	2.02	0.58
1:A:306:PHE:CZ	1:A:316:GLY:O	2.58	0.57
1:B:334:LYS:NZ	5:B:596:HOH:O	2.36	0.56
1:D:115:LEU:HD23	1:D:329:PRO:HB2	1.87	0.56
1:C:214:LEU:HD11	1:C:229:LEU:HB3	1.86	0.56
1:D:125:TRP:CD2	1:D:355:ALA:HB2	2.40	0.55
1:C:277:GLU:OE1	1:C:277:GLU:N	2.28	0.55
1:A:275:ARG:HD3	1:A:319:MET:HE2	1.88	0.55
1:A:275:ARG:HB2	1:A:277:GLU:CD	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:PHE:CE2	1:C:316:GLY:C	2.85	0.55
1:D:340:ARG:HG2	1:D:354:TRP:CD2	2.42	0.54
1:B:332:LYS:NZ	1:D:277:GLU:OE1	2.40	0.54
2:D:405:EDO:H21	5:D:588:HOH:O	2.07	0.54
1:C:171:GLN:NE2	5:C:597:HOH:O	2.40	0.53
1:C:319:MET:HA	1:C:319:MET:HE2	1.91	0.53
1:C:183:CYS:HB3	5:C:643:HOH:O	2.09	0.52
1:A:125:TRP:CD2	1:A:355:ALA:HB2	2.44	0.52
1:D:240:ARG:NH1	1:D:277:GLU:OE2	2.43	0.52
1:A:253:LYS:HZ2	1:A:257:ILE:HD11	1.73	0.52
1:A:275:ARG:HD3	1:A:319:MET:CE	2.40	0.51
1:B:125:TRP:CD2	1:B:355:ALA:HB2	2.46	0.51
1:B:275:ARG:HD3	1:B:319:MET:CE	2.40	0.51
1:D:240:ARG:HH21	1:D:275:ARG:HG3	1.75	0.51
1:D:277:GLU:HG2	5:D:555:HOH:O	2.11	0.50
1:B:275:ARG:HB2	1:B:277:GLU:OE2	2.12	0.49
1:C:210:MET:HE3	1:C:234:GLU:CG	2.41	0.49
1:D:240:ARG:NH2	1:D:275:ARG:HG3	2.27	0.49
1:A:306:PHE:CD2	1:A:318:LYS:HG3	2.48	0.48
1:C:255:ARG:CZ	1:C:283:PRO:HG3	2.44	0.48
1:A:239:HIS:HD2	1:A:242:GLN:HE22	1.60	0.48
1:A:311:LYS:HE2	5:A:637:HOH:O	2.14	0.48
1:A:128:ASP:HB3	1:A:138:ARG:NH2	2.29	0.47
1:B:194:MET:SD	1:C:181:LYS:HE2	2.54	0.47
1:D:113:GLU:N	1:D:116:LYS:CG	2.68	0.47
1:A:280:SER:OG	1:A:281:ARG:N	2.43	0.47
1:B:113:GLU:CG	1:B:114:ASP:N	2.45	0.47
1:B:328:GLY:N	2:B:405:EDO:H21	2.24	0.47
1:B:275:ARG:HG2	1:B:278:GLU:CD	2.40	0.46
1:B:277:GLU:H	1:B:277:GLU:CD	2.15	0.46
1:C:235:SER:C	1:C:236:THR:HG23	2.41	0.46
1:A:340:ARG:HG2	1:A:354:TRP:CD2	2.51	0.46
1:B:158:GLU:OE2	4:B:404:MLI:O7	2.34	0.46
1:A:332:LYS:CE	1:A:362:ALA:O	2.64	0.45
1:B:212:ARG:HD2	1:B:232:HIS:O	2.16	0.45
1:D:150:ASN:O	2:D:405:EDO:H11	2.15	0.45
1:C:304:ASP:OD1	1:C:306:PHE:HB2	2.16	0.45
1:C:180:ASN:CG	1:C:183:CYS:SG	3.00	0.45
1:D:121:SER:OG	1:D:151:PRO:HA	2.15	0.45
1:D:125:TRP:CG	1:D:355:ALA:HB2	2.51	0.45
1:B:328:GLY:H	2:B:405:EDO:C2	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:PHE:CZ	1:A:316:GLY:C	2.95	0.44
1:C:198:GLU:OE1	1:C:225:LYS:NZ	2.43	0.44
1:C:252:ASP:O	1:C:256:GLU:HG3	2.18	0.44
1:D:240:ARG:N	1:D:241:PRO:CD	2.80	0.44
2:B:405:EDO:H22	5:B:647:HOH:O	2.17	0.44
1:C:282:VAL:HA	1:C:283:PRO:HD3	1.75	0.44
1:D:332:LYS:HE2	1:D:362:ALA:C	2.43	0.44
1:A:114:ASP:HA	2:A:406:EDO:H21	1.99	0.44
1:A:306:PHE:CE2	1:A:316:GLY:O	2.70	0.44
1:C:340:ARG:HG2	1:C:354:TRP:CD2	2.52	0.44
1:D:115:LEU:HD12	1:D:115:LEU:HA	1.47	0.44
1:C:147:LYS:NZ	5:C:584:HOH:O	2.51	0.43
1:B:240:ARG:HH21	1:B:275:ARG:HG3	1.83	0.43
1:C:125:TRP:CG	1:C:355:ALA:HB2	2.53	0.43
1:D:214:LEU:HD11	1:D:229:LEU:HB3	2.01	0.43
1:B:275:ARG:HB2	1:B:277:GLU:CD	2.44	0.43
1:B:190:LEU:HD12	1:B:190:LEU:N	2.35	0.42
1:D:240:ARG:HB3	1:D:241:PRO:HD3	2.00	0.42
1:C:314:PHE:C	1:C:315:HIS:ND1	2.78	0.42
1:D:221:ILE:HG22	1:D:226:VAL:HG21	1.99	0.42
1:D:282:VAL:HA	1:D:283:PRO:HD3	1.80	0.42
1:B:328:GLY:O	2:B:405:EDO:H21	2.20	0.42
1:B:311:LYS:HE2	1:B:352:ASP:OD2	2.19	0.42
1:A:306:PHE:CZ	1:A:316:GLY:CA	3.03	0.42
1:A:235:SER:C	1:A:236:THR:HG23	2.46	0.41
1:C:318:LYS:C	1:C:319:MET:HG2	2.44	0.41
1:A:240:ARG:N	1:A:241:PRO:CD	2.82	0.41
1:C:210:MET:HE3	1:C:234:GLU:CD	2.45	0.41
1:C:275:ARG:HG2	1:C:275:ARG:H	1.56	0.41
1:C:158:GLU:OE2	4:C:402:MLI:O8	2.38	0.41
1:C:240:ARG:N	1:C:241:PRO:CD	2.83	0.41
1:B:280:SER:OG	1:B:281:ARG:N	2.54	0.41
1:D:275:ARG:HG2	1:D:275:ARG:H	1.73	0.40
1:B:303:TRP:HZ2	1:B:311:LYS:HZ1	1.66	0.40
1:B:214:LEU:HD11	1:B:229:LEU:HB3	2.03	0.40
1:B:235:SER:C	1:B:236:THR:HG23	2.46	0.40
1:C:113:GLU:O	1:C:113:GLU:HG2	2.20	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	247/256 (96%)	241 (98%)	6 (2%)	0	100	100
1	B	248/256 (97%)	244 (98%)	4 (2%)	0	100	100
1	C	249/256 (97%)	244 (98%)	5 (2%)	0	100	100
1	D	244/256 (95%)	240 (98%)	4 (2%)	0	100	100
All	All	988/1024 (96%)	969 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	217/221 (98%)	213 (98%)	4 (2%)	51	51
1	B	218/221 (99%)	216 (99%)	2 (1%)	70	74
1	C	218/221 (99%)	214 (98%)	4 (2%)	51	51
1	D	216/221 (98%)	212 (98%)	4 (2%)	50	49
All	All	869/884 (98%)	855 (98%)	14 (2%)	55	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ILE
1	A	275	ARG

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Mol	Chain	Res	Type
1	A	326	TRP
1	A	331	ASP
1	B	275	ARG
1	B	326	TRP
1	C	275	ARG
1	C	307	LYS
1	C	319	MET
1	C	326	TRP
1	D	115	LEU
1	D	275	ARG
1	D	326	TRP
1	D	344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	206	GLN
1	A	239	HIS
1	A	261	ASN
1	B	260	GLN
1	B	312	GLN
1	C	180	ASN
1	D	171	GLN
1	D	215	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	MLI	A	403	3	6,6,6	1.28	0	7,7,7	1.26	0
4	MLI	B	406	-	6,6,6	1.19	0	7,7,7	1.20	0
2	EDO	A	406	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	C	405	-	3,3,3	0.46	0	2,2,2	0.30	0
4	MLI	C	402	3	6,6,6	1.21	0	7,7,7	1.06	0
2	EDO	B	408	-	3,3,3	0.54	0	2,2,2	0.16	0
2	EDO	A	401	-	3,3,3	0.53	0	2,2,2	0.35	0
2	EDO	D	403	-	3,3,3	0.52	0	2,2,2	0.29	0
4	MLI	D	402	3	6,6,6	1.34	0	7,7,7	1.18	1 (14%)
2	EDO	C	406	-	3,3,3	0.44	0	2,2,2	0.35	0
2	EDO	B	405	-	3,3,3	0.41	0	2,2,2	0.36	0
2	EDO	A	404	-	3,3,3	0.42	0	2,2,2	0.43	0
2	EDO	B	402	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	B	407	-	3,3,3	0.49	0	2,2,2	0.14	0
2	EDO	C	403	-	3,3,3	0.53	0	2,2,2	0.28	0
2	EDO	D	405	-	3,3,3	0.45	0	2,2,2	0.26	0
2	EDO	D	404	-	3,3,3	0.58	0	2,2,2	0.14	0
2	EDO	C	404	-	3,3,3	0.47	0	2,2,2	0.27	0
4	MLI	B	404	3	6,6,6	1.33	0	7,7,7	1.32	1 (14%)
2	EDO	A	405	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	B	401	-	3,3,3	0.45	0	2,2,2	0.40	0
2	EDO	B	409	-	3,3,3	0.47	0	2,2,2	0.28	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	MLI	A	403	3	-	0/4/4/4	-
4	MLI	B	406	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	406	-	-	0/1/1/1	-
2	EDO	C	405	-	-	1/1/1/1	-
4	MLI	C	402	3	-	0/4/4/4	-
2	EDO	B	408	-	-	1/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	D	403	-	-	0/1/1/1	-
4	MLI	D	402	3	-	0/4/4/4	-
2	EDO	C	406	-	-	0/1/1/1	-
2	EDO	B	405	-	-	0/1/1/1	-
2	EDO	A	404	-	-	1/1/1/1	-
2	EDO	B	402	-	-	1/1/1/1	-
2	EDO	B	407	-	-	0/1/1/1	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
2	EDO	D	404	-	-	1/1/1/1	-
2	EDO	C	404	-	-	1/1/1/1	-
4	MLI	B	404	3	-	0/4/4/4	-
2	EDO	A	405	-	-	1/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	B	409	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	MLI	O9-C3-C1	2.09	120.98	114.51
4	D	402	MLI	O9-C3-C1	2.05	120.87	114.51

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	408	EDO	O1-C1-C2-O2
2	B	409	EDO	O1-C1-C2-O2
2	C	404	EDO	O1-C1-C2-O2
2	C	405	EDO	O1-C1-C2-O2
2	D	405	EDO	O1-C1-C2-O2
2	A	405	EDO	O1-C1-C2-O2
2	A	401	EDO	O1-C1-C2-O2
2	A	404	EDO	O1-C1-C2-O2
2	B	402	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	404	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	406	EDO	1	0
4	C	402	MLI	1	0
2	B	405	EDO	5	0
2	B	407	EDO	1	0
2	D	405	EDO	2	0
4	B	404	MLI	1	0
2	A	405	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	249/256 (97%)	-0.15	5 (2%) 65 67	18, 28, 65, 94	0
1	B	250/256 (97%)	-0.19	3 (1%) 76 78	17, 26, 59, 81	0
1	C	251/256 (98%)	-0.13	7 (2%) 55 56	17, 28, 68, 124	0
1	D	248/256 (96%)	-0.16	2 (0%) 82 84	18, 30, 54, 92	0
All	All	998/1024 (97%)	-0.16	17 (1%) 69 71	17, 28, 64, 124	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	GLY	4.7
1	A	316	GLY	3.3
1	C	112	ALA	3.2
1	D	313	GLY	2.9
1	C	315	HIS	2.7
1	A	306	PHE	2.7
1	B	281	ARG	2.5
1	A	315	HIS	2.4
1	C	316	GLY	2.3
1	B	315	HIS	2.3
1	C	314	PHE	2.3
1	C	182	GLY	2.3
1	C	211	TYR	2.3
1	B	312	GLN	2.1
1	C	312	GLN	2.1
1	D	316	GLY	2.1
1	A	222	GLY	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	EDO	A	405	4/4	0.38	0.24	77,92,94,97	0
2	EDO	A	406	4/4	0.58	0.16	65,78,81,84	0
2	EDO	B	407	4/4	0.62	0.23	70,84,86,88	0
2	EDO	C	404	4/4	0.64	0.18	63,76,77,84	0
2	EDO	B	402	4/4	0.65	0.16	71,85,85,89	0
2	EDO	A	404	4/4	0.69	0.18	56,67,74,82	0
2	EDO	C	405	4/4	0.70	0.17	78,94,96,96	0
2	EDO	D	405	4/4	0.72	0.12	67,80,81,85	0
2	EDO	A	401	4/4	0.73	0.14	36,44,52,62	0
4	MLI	B	406	7/7	0.75	0.15	45,65,78,78	0
2	EDO	C	406	4/4	0.78	0.18	71,86,87,90	0
2	EDO	D	404	4/4	0.78	0.14	45,62,72,74	0
2	EDO	B	405	4/4	0.79	0.11	54,65,67,68	0
2	EDO	B	409	4/4	0.79	0.16	64,77,84,90	0
2	EDO	B	401	4/4	0.81	0.11	37,45,51,57	0
2	EDO	B	408	4/4	0.83	0.14	44,55,65,66	0
2	EDO	C	403	4/4	0.83	0.12	43,51,58,58	0
2	EDO	D	403	4/4	0.84	0.10	39,46,48,48	0
4	MLI	C	402	7/7	0.91	0.09	30,37,48,48	0
4	MLI	D	402	7/7	0.92	0.09	26,30,39,42	0
4	MLI	A	403	7/7	0.93	0.07	28,31,37,39	0
3	MG	C	401	1/1	0.96	0.10	39,39,39,39	0
4	MLI	B	404	7/7	0.97	0.05	26,31,38,40	0
3	MG	B	403	1/1	0.97	0.15	28,28,28,28	0
3	MG	D	401	1/1	0.98	0.04	33,33,33,33	0
3	MG	A	402	1/1	0.98	0.09	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.