Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:20 AM BST

PDB ID	:	6YG1
Title	:	Crystal structure of MKK7 (MAP2K7) in an active state, allosterically triggered by the N-terminal helix
Authors	:	Chaikuad, A.; Knapp, S.; Structural Genomics Consortium (SGC); Scottish Structural Proteomics Facility (SSPF)
Deposited on	:	2020-03-27
Resolution	:	2.22 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 following versions of software and data (see references ⓘ) were used in the production of this report:

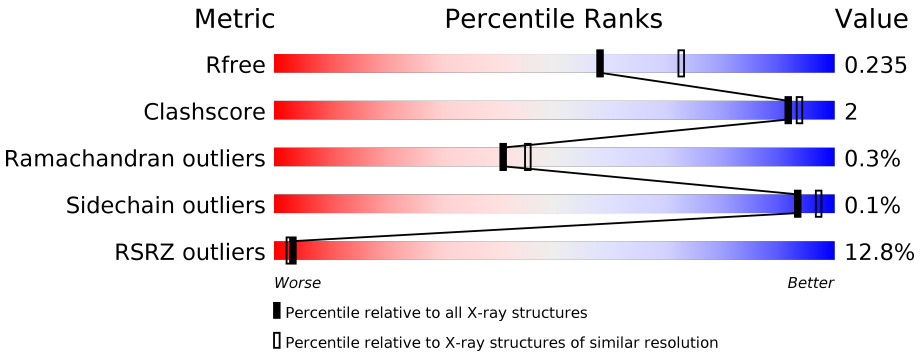
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 on 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	348	2% 85% 5% 10%
1	B	348	14% 85% • 12%
1	C	348	18% 87% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7697 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 Dual specificity mitogen-activated protein kinase kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	3	0
			2524	1605	434	465	20			
1	B	307	Total	C	N	O	S	0	1	0
			2375	1516	408	435	16			
1	C	315	Total	C	N	O	S	0	1	0
			2445	1557	418	453	17			

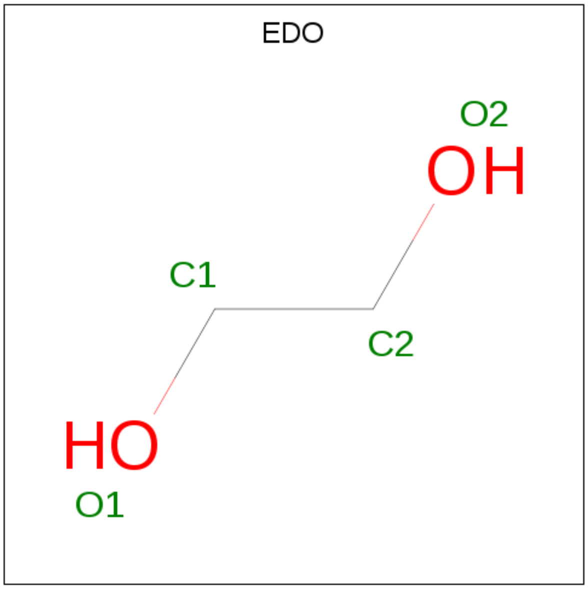
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	SER	-	expression tag	UNP O14733
A	75	MET	-	expression tag	UNP O14733
A	287	ASP	SER	engineered mutation	UNP O14733
A	291	ASP	THR	engineered mutation	UNP O14733
B	74	SER	-	expression tag	UNP O14733
B	75	MET	-	expression tag	UNP O14733
B	287	ASP	SER	engineered mutation	UNP O14733
B	291	ASP	THR	engineered mutation	UNP O14733
C	74	SER	-	expression tag	UNP O14733
C	75	MET	-	expression tag	UNP O14733
C	287	ASP	SER	engineered mutation	UNP O14733
C	291	ASP	THR	engineered mutation	UNP O14733

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 4 is water.

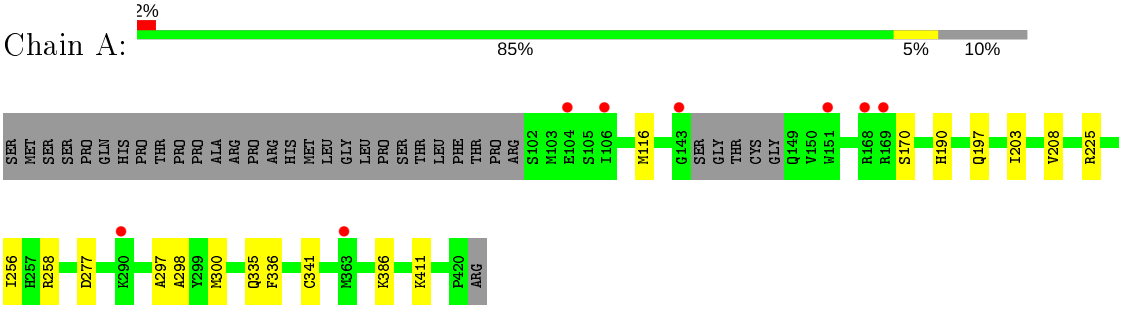
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	147	Total O 147 147	0	0
4	B	64	Total O 64 64	0	0
4	C	46	Total O 46 46	0	0

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.

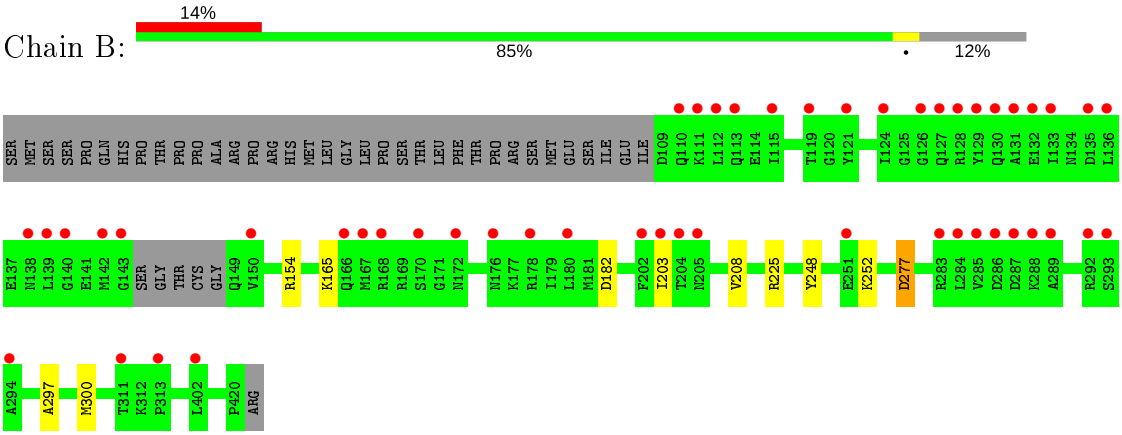
- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 7

Chain A:



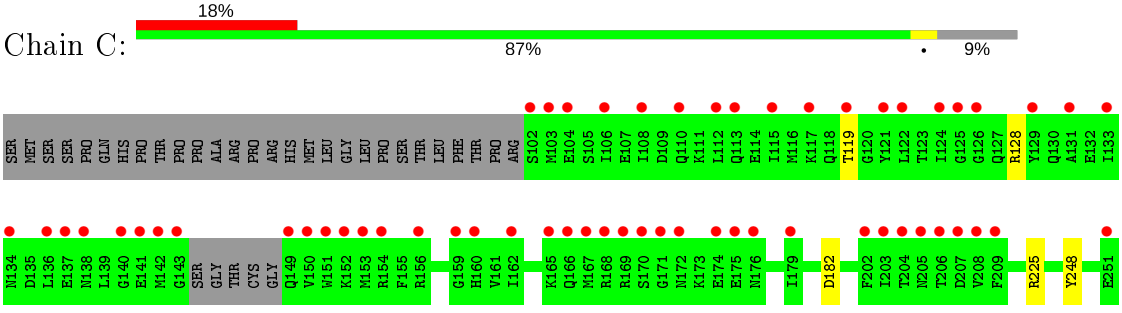
- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 7

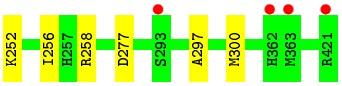
Chain B:



- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 7

Chain C:




K252
I256
H257
R258
D277
S293
A297
M300
H362
M363
R421

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.16Å 67.87Å 142.78Å 90.00° 114.76° 90.00°	Depositor
Resolution (Å)	64.83 – 2.22 58.51 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.83-2.22) 99.8 (58.51-2.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.204 , 0.232 0.208 , 0.235	Depositor DCC
R_{free} test set	2724 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7697	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 4.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.74	0/2581	0.76	2/3470 (0.1%)
1	B	0.65	0/2426	0.73	3/3278 (0.1%)
1	C	0.63	0/2496	0.76	5/3369 (0.1%)
All	All	0.68	0/7503	0.75	10/10117 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	225	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	C	128	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	B	225	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	225	ARG	NE-CZ-NH1	-6.91	116.84	120.30
1	C	225	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	B	225	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	A	225	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	C	128	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	154	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	C	182	ASP	CB-CG-OD1	5.04	122.83	118.30

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	2524	0	2558	12	0
1	B	2375	0	2329	8	0
1	C	2445	0	2391	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
3	A	68	0	102	2	0
3	B	20	0	30	0	0
3	C	4	0	6	0	0
4	A	147	0	0	2	0
4	B	64	0	0	4	0
4	C	46	0	0	0	0
All	All	7697	0	7416	23	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 (23) 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:182:ASP:HB2	4:B:613:HOH:O	1.83	0.78
1:A:386:LYS:HB3	3:A:505:EDO:H22	1.76	0.68
1:A:190:HIS:CE1	1:A:197:GLN:HE21	2.16	0.62
1:A:341:CYS:SG	3:A:515:EDO:H22	2.45	0.56
1:A:116:MET:SD	1:A:203:ILE:HG21	2.46	0.55
1:B:248:TYR:CD1	1:B:252:LYS:HG3	2.43	0.53
1:C:248:TYR:CD2	1:C:252:LYS:HG3	2.48	0.49
1:A:298:ALA:HB1	1:A:336:PHE:CZ	2.49	0.47
1:A:411:LYS:NZ	4:A:601:HOH:O	2.34	0.47
1:B:165:LYS:NZ	4:B:603:HOH:O	2.48	0.46
1:B:248:TYR:CE1	1:B:252:LYS:HG3	2.51	0.46
1:A:190:HIS:CE1	1:A:197:GLN:NE2	2.84	0.45
1:B:165:LYS:HD3	4:B:602:HOH:O	2.16	0.45
1:A:297:ALA:HA	1:A:300:MET:HG3	1.98	0.44
1:A:203:ILE:HG22	1:A:208:VAL:HG22	1.99	0.43
1:A:256:ILE:HG12	1:A:258:ARG:HG3	2.00	0.43
1:B:277:ASP:HA	4:B:613:HOH:O	2.19	0.42
1:C:297:ALA:HA	1:C:300:MET:HG3	2.01	0.42
1:B:203:ILE:HG22	1:B:208:VAL:HG22	2.02	0.42
1:A:335[A]:GLN:NE2	4:A:604:HOH:O	2.48	0.41
1:B:297:ALA:HA	1:B:300:MET:HG3	2.03	0.41
1:C:256:ILE:HG12	1:C:258:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:O	1:A:170:SER:OG	2.31	0.41

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	313/348 (90%)	307 (98%)	5 (2%)	1 (0%)	41	45
1	B	304/348 (87%)	298 (98%)	5 (2%)	1 (0%)	41	45
1	C	312/348 (90%)	306 (98%)	5 (2%)	1 (0%)	41	45
All	All	929/1044 (89%)	911 (98%)	15 (2%)	3 (0%)	41	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASP
1	C	277	ASP
1	B	277	ASP

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	278/308 (90%)	278 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	247/308 (80%)	247 (100%)	0	100 100
1	C	255/308 (83%)	254 (100%)	1 (0%)	91 95
All	All	780/924 (84%)	779 (100%)	1 (0%)	93 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	119	THR

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

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 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
3	EDO	A	504	-	3,3,3	0.58	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	A	508	-	3,3,3	0.57	0	2,2,2	0.14	0
3	EDO	A	516	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	A	505	-	3,3,3	0.59	0	2,2,2	0.36	0
3	EDO	A	509	-	3,3,3	0.59	0	2,2,2	0.10	0
3	EDO	A	514	-	3,3,3	0.46	0	2,2,2	0.29	0
3	EDO	B	506	-	3,3,3	0.42	0	2,2,2	0.19	0
3	EDO	A	517	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	A	515	-	3,3,3	0.56	0	2,2,2	0.60	0
3	EDO	A	511	-	3,3,3	0.57	0	2,2,2	0.26	0
3	EDO	A	507	-	3,3,3	0.67	0	2,2,2	0.22	0
3	EDO	B	505	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	A	513	-	3,3,3	0.61	0	2,2,2	0.22	0
3	EDO	A	512	-	3,3,3	0.39	0	2,2,2	0.16	0
3	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.31	0
3	EDO	A	518	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	B	503	-	3,3,3	0.48	0	2,2,2	0.13	0
3	EDO	A	502	-	3,3,3	0.40	0	2,2,2	0.36	0
3	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.23	0
3	EDO	A	506	-	3,3,3	0.70	0	2,2,2	0.39	0
3	EDO	A	510	-	3,3,3	0.41	0	2,2,2	0.35	0
3	EDO	C	503	-	3,3,3	0.48	0	2,2,2	0.50	0
3	EDO	B	504	-	3,3,3	0.37	0	2,2,2	0.25	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
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	A	516	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
3	EDO	B	506	-	-	1/1/1/1	-
3	EDO	A	517	-	-	1/1/1/1	-
3	EDO	A	515	-	-	1/1/1/1	-
3	EDO	A	511	-	-	1/1/1/1	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	A	518	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	516	EDO	O1-C1-C2-O2
3	A	517	EDO	O1-C1-C2-O2
3	B	505	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
3	A	508	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2
3	A	509	EDO	O1-C1-C2-O2
3	B	506	EDO	O1-C1-C2-O2
3	A	515	EDO	O1-C1-C2-O2
3	A	518	EDO	O1-C1-C2-O2
3	A	506	EDO	O1-C1-C2-O2
3	A	511	EDO	O1-C1-C2-O2
3	A	513	EDO	O1-C1-C2-O2
3	A	510	EDO	O1-C1-C2-O2
3	B	504	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	EDO	1	0
3	A	515	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

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, 95^{th} 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	314/348 (90%)	0.16	8 (2%) 57 55	22, 44, 101, 126	0
1	B	307/348 (88%)	0.72	50 (16%) 1 1	28, 63, 134, 156	0
1	C	315/348 (90%)	0.85	62 (19%) 1 1	38, 62, 129, 157	0
All	All	936/1044 (89%)	0.57	120 (12%) 3 3	22, 57, 126, 157	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	125	GLY	8.9
1	B	294	ALA	8.5
1	B	287	ASP	8.3
1	C	209	PHE	8.2
1	C	170	SER	8.1
1	B	111	LYS	7.8
1	C	202	PHE	7.3
1	C	129	TYR	7.3
1	C	124	ILE	7.0
1	C	206	THR	6.7
1	C	106	ILE	6.7
1	C	151	TRP	6.5
1	B	121	TYR	6.5
1	B	143	GLY	6.3
1	C	115	ILE	6.2
1	B	202	PHE	6.1
1	B	170	SER	6.1
1	C	169	ARG	6.0
1	C	133	ILE	5.9
1	C	203	ILE	5.9
1	C	134	ASN	5.8
1	B	203	ILE	5.7
1	B	285	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	286	ASP	5.5
1	C	166	GLN	5.1
1	B	150	VAL	5.1
1	C	142	MET	5.1
1	C	172	ASN	4.9
1	C	113	GLN	4.9
1	C	208	VAL	4.7
1	B	139	LEU	4.7
1	C	167	MET	4.6
1	C	121	TYR	4.6
1	C	150	VAL	4.5
1	C	112	LEU	4.3
1	C	126	GLY	4.2
1	B	115	ILE	4.1
1	B	133	ILE	4.1
1	C	131	ALA	4.0
1	C	204	THR	3.9
1	B	176	ASN	3.9
1	B	289	ALA	3.9
1	B	127	GLN	3.9
1	B	284	LEU	3.8
1	C	136	LEU	3.8
1	C	165	LYS	3.8
1	C	176	ASN	3.7
1	C	141	GLU	3.7
1	B	142	MET	3.7
1	C	205	ASN	3.6
1	C	110	GLN	3.6
1	C	149	GLN	3.6
1	B	112	LEU	3.5
1	B	130	GLN	3.5
1	B	283	ARG	3.5
1	C	152	LYS	3.5
1	C	117	LYS	3.4
1	B	110	GLN	3.4
1	B	126	GLY	3.4
1	C	168	ARG	3.4
1	B	167	MET	3.4
1	C	362	HIS	3.3
1	C	159	GLY	3.3
1	B	205	ASN	3.2
1	B	128	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLY	3.1
1	B	311	THR	3.1
1	C	179	ILE	3.1
1	C	103	MET	3.1
1	C	174	GLU	3.0
1	A	169	ARG	3.0
1	B	288	LYS	3.0
1	B	166	GLN	3.0
1	B	293	SER	2.9
1	B	204	THR	2.9
1	C	421	ARG	2.8
1	C	143	GLY	2.8
1	C	102	SER	2.8
1	C	153	MET	2.8
1	A	143	GLY	2.7
1	C	154	ARG	2.7
1	C	207	ASP	2.7
1	B	172	ASN	2.7
1	C	156	ARG	2.6
1	C	122	LEU	2.6
1	C	104	GLU	2.6
1	B	178	ARG	2.6
1	B	129	TYR	2.6
1	C	171	GLY	2.6
1	B	132	GLU	2.5
1	C	119	THR	2.5
1	C	138	ASN	2.5
1	C	108	ILE	2.4
1	C	160	HIS	2.4
1	C	175	GLU	2.4
1	C	162	ILE	2.4
1	B	180	LEU	2.4
1	B	138	ASN	2.3
1	A	168	ARG	2.3
1	B	292	ARG	2.3
1	B	168	ARG	2.3
1	A	104	GLU	2.2
1	B	124	ILE	2.2
1	B	135	ASP	2.2
1	A	363[A]	MET	2.2
1	B	131	ALA	2.2
1	A	106	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	2.2
1	A	151	TRP	2.2
1	B	113	GLN	2.2
1	C	293	SER	2.1
1	A	290	LYS	2.1
1	B	402	LEU	2.1
1	B	251	GLU	2.1
1	B	119	THR	2.1
1	C	251	GLU	2.1
1	C	140	GLY	2.1
1	B	313	PRO	2.1
1	C	137	GLU	2.0
1	C	363	MET	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, 95^{th} 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
3	EDO	A	511	4/4	0.62	0.20	73,75,76,78	0
3	EDO	A	509	4/4	0.75	0.16	76,79,79,80	0
3	EDO	A	513	4/4	0.76	0.19	66,66,68,69	0
3	EDO	A	506	4/4	0.77	0.22	49,57,59,62	0
3	EDO	A	516	4/4	0.79	0.16	67,69,70,70	0
3	EDO	C	503	4/4	0.79	0.37	57,61,69,75	0
3	EDO	A	508	4/4	0.81	0.15	67,73,74,74	0
3	EDO	A	517	4/4	0.81	0.12	66,66,68,69	0
3	EDO	B	503	4/4	0.82	0.17	63,68,71,73	0
3	EDO	A	514	4/4	0.82	0.14	83,83,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	503	4/4	0.82	0.14	70,72,73,79	0
3	EDO	B	506	4/4	0.85	0.23	51,52,56,65	0
3	EDO	B	504	4/4	0.85	0.29	61,65,68,68	0
3	EDO	A	507	4/4	0.86	0.28	54,60,60,67	0
3	EDO	A	504	4/4	0.87	0.17	61,64,64,67	0
3	EDO	A	505	4/4	0.88	0.35	43,43,52,63	0
3	EDO	A	515	4/4	0.88	0.36	34,35,42,55	0
3	EDO	A	518	4/4	0.90	0.13	71,72,73,75	0
3	EDO	A	510	4/4	0.90	0.15	65,65,68,70	0
3	EDO	A	512	4/4	0.91	0.25	55,55,61,62	4
3	EDO	B	502	4/4	0.91	0.20	59,60,61,70	0
2	NA	C	501	1/1	0.93	0.11	48,48,48,48	0
3	EDO	A	502	4/4	0.94	0.19	45,51,55,65	0
3	EDO	B	505	4/4	0.95	0.13	67,72,72,73	0
2	NA	B	501	1/1	0.97	0.07	51,51,51,51	0
2	NA	C	502	1/1	0.97	0.06	39,39,39,39	1
2	NA	A	501	1/1	0.98	0.20	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.