



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2021 – 03:12 am BST

PDB ID : 7AHS  
Title : titin-N2A Ig81-Ig83  
Authors : Fleming, J.R.; Mayans, O.  
Deposited on : 2020-09-25  
Resolution : 2.05 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](mailto: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.

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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 : 2.18  
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) : 2.18

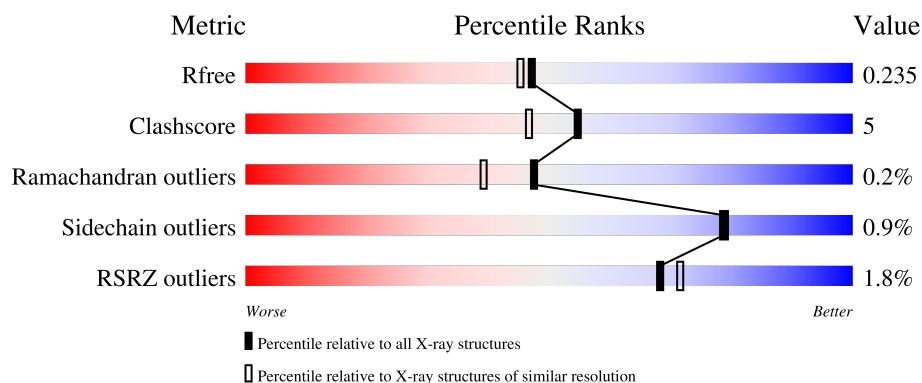
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	273	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="width: 100%; height: 10px; background-color: red;"></div> </div>
1	B	273	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 89%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: red;"></div> </div>
1	C	273	<div> <div style="width: 89%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="width: 100%; height: 10px; background-color: red;"></div> </div>
1	D	273	<div> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 18%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: red;"></div> </div>

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	D	306	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9852 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 Isoform 5 of Titin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	3	1	0
			2200	1380	382	429	9			
1	B	272	Total	C	N	O	S	0	0	0
			2205	1383	383	429	10			
1	C	271	Total	C	N	O	S	0	0	0
			2197	1378	382	428	9			
1	D	272	Total	C	N	O	S	3	1	0
			2208	1385	383	430	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8WZ42
A	-1	ALA	-	expression tag	UNP Q8WZ42
A	0	MET	-	expression tag	UNP Q8WZ42
B	-2	GLY	-	expression tag	UNP Q8WZ42
B	-1	ALA	-	expression tag	UNP Q8WZ42
B	0	MET	-	expression tag	UNP Q8WZ42
C	-2	GLY	-	expression tag	UNP Q8WZ42
C	-1	ALA	-	expression tag	UNP Q8WZ42
C	0	MET	-	expression tag	UNP Q8WZ42
D	-2	GLY	-	expression tag	UNP Q8WZ42
D	-1	ALA	-	expression tag	UNP Q8WZ42
D	0	MET	-	expression tag	UNP Q8WZ42

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



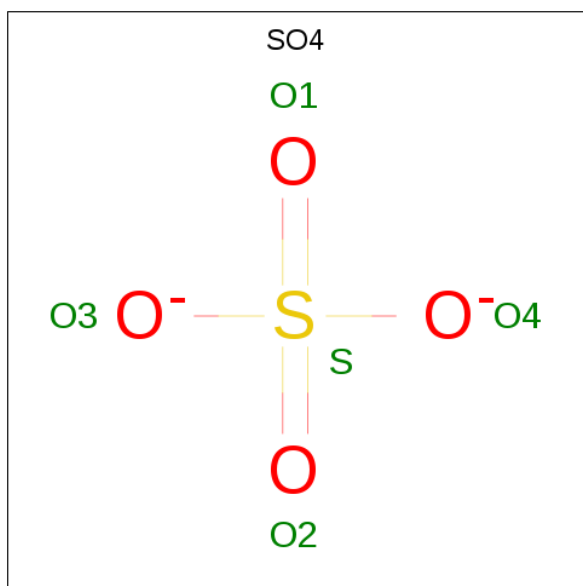
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



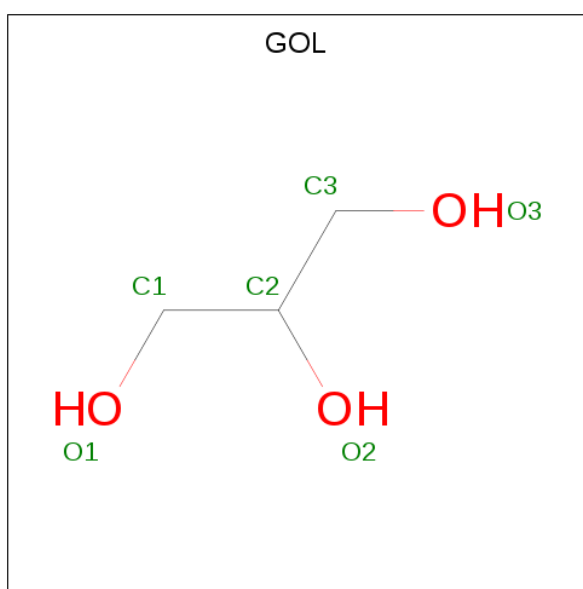
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	240	Total	O	0	0
			240	240		
5	B	292	Total	O	0	0
			292	292		
5	C	227	Total	O	0	0
			227	227		
5	D	151	Total	O	0	0
			151	151		

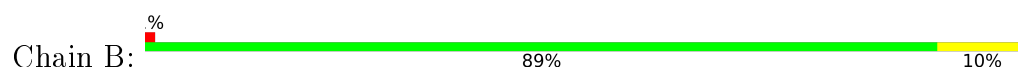
### 3 Residue-property plots [i](#)

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.

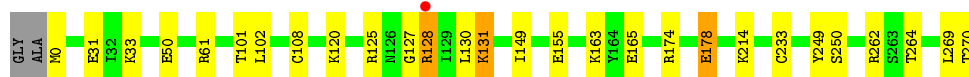
- Molecule 1: Isoform 5 of Titin



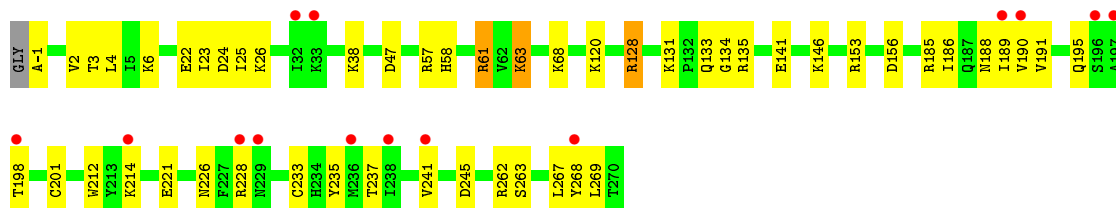
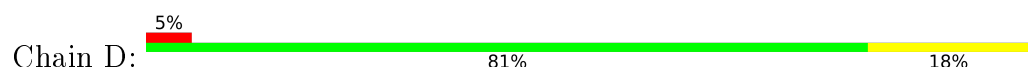
- Molecule 1: Isoform 5 of Titin



- Molecule 1: Isoform 5 of Titin



- Molecule 1: Isoform 5 of Titin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.20Å 87.34Å 161.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.53 – 2.05 48.68 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.53-2.05) 91.6 (48.68-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.183 , 0.235 0.183 , 0.235	Depositor DCC
$R_{free}$ test set	1840 reflections (2.41%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: EDO, SO4, GOL

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	0.44	1/2248 (0.0%)	0.68	5/3045 (0.2%)
1	B	0.48	1/2250 (0.0%)	0.63	1/3047 (0.0%)
1	C	0.44	0/2242	0.70	5/3037 (0.2%)
1	D	0.49	3/2256 (0.1%)	0.82	12/3055 (0.4%)
All	All	0.46	5/8996 (0.1%)	0.71	23/12184 (0.2%)

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	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	LYS	CE-NZ	6.12	1.64	1.49
1	A	6	LYS	CE-NZ	5.86	1.63	1.49
1	D	6	LYS	CD-CE	5.82	1.65	1.51
1	D	120	LYS	CD-CE	5.77	1.65	1.51
1	B	184	LYS	CD-CE	5.36	1.64	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	ARG	NE-CZ-NH1	-15.14	112.73	120.30
1	D	128	ARG	CD-NE-CZ	10.37	138.12	123.60
1	A	6	LYS	CA-CB-CG	10.11	135.65	113.40
1	D	6	LYS	CB-CG-CD	9.01	135.03	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	GLU	CA-CB-CG	-8.79	94.06	113.40
1	A	6	LYS	N-CA-CB	8.58	126.04	110.60
1	A	6	LYS	CG-CD-CE	-7.06	90.72	111.90
1	D	120	LYS	CD-CE-NZ	6.82	127.39	111.70
1	C	128	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	D	120	LYS	CG-CD-CE	-6.62	92.05	111.90
1	D	214	LYS	CA-CB-CG	6.47	127.64	113.40
1	D	6	LYS	CA-CB-CG	-6.30	99.54	113.40
1	C	128	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	33	LYS	CB-CG-CD	-6.15	95.60	111.60
1	A	6	LYS	CB-CA-C	-6.13	98.14	110.40
1	D	63	LYS	CD-CE-NZ	-5.72	98.53	111.70
1	D	228	ARG	CG-CD-NE	5.60	123.56	111.80
1	D	63	LYS	CB-CG-CD	-5.40	97.56	111.60
1	D	6	LYS	CG-CD-CE	-5.39	95.72	111.90
1	D	61	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	A	6	LYS	CB-CG-CD	5.38	125.58	111.60
1	B	178	GLU	CA-CB-CG	5.34	125.15	113.40
1	C	128	ARG	CD-NE-CZ	5.07	130.70	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	128	ARG	Sidechain

## 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	2200	0	2157	13	0
1	B	2205	0	2164	25	0
1	C	2197	0	2152	23	0
1	D	2208	0	2169	31	3
2	A	20	0	30	0	0
2	B	28	0	42	1	0
2	C	12	0	18	2	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	16	0	24	0	0
3	B	30	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	0	0
4	C	6	0	8	0	0
5	A	240	0	0	4	2
5	B	292	0	0	7	3
5	C	227	0	0	7	3
5	D	151	0	0	5	2
All	All	9852	0	8764	91	8

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 5.

All (91) 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:184:LYS:NZ	1:B:202:GLU:OE1	1.91	1.02
1:D:131:LYS:HB3	1:D:133:GLN:HG2	1.50	0.92
1:C:233:CYS:SG	5:C:574:HOH:O	2.32	0.84
1:C:0:MET:N	5:C:402:HOH:O	2.15	0.80
1:B:233:CYS:SG	5:B:599:HOH:O	2.41	0.79
1:A:146:LYS:NZ	5:A:402:HOH:O	2.18	0.77
1:B:150:ALA:N	5:B:402:HOH:O	2.17	0.76
1:D:153:ARG:NH1	5:D:401:HOH:O	2.22	0.73
1:C:131:LYS:H	1:C:131:LYS:HD3	1.54	0.72
1:C:269:LEU:O	1:C:270:THR:HB	1.91	0.71
1:D:233:CYS:SG	5:D:540:HOH:O	2.49	0.70
1:D:191:VAL:HG13	1:D:195:GLN:HB3	1.74	0.69
1:B:184:LYS:HB2	1:B:202:GLU:HB3	1.75	0.69
1:A:7:ASP:OD1	5:A:401:HOH:O	2.10	0.69
1:D:131:LYS:O	1:D:133:GLN:HG3	1.93	0.68
1:C:155:GLU:OE2	5:C:401:HOH:O	2.12	0.68
1:D:61:ARG:HD3	1:D:63:LYS:NZ	2.08	0.67
1:B:131:LYS:HE2	1:B:133:GLN:HB3	1.79	0.64
1:B:131:LYS:HE2	1:B:133:GLN:CB	2.28	0.64
1:D:198:THR:OG1	1:D:237:THR:HG22	2.00	0.62
1:A:214:LYS:HD2	1:A:249:TYR:CZ	2.35	0.61
1:B:118:ASN:HB3	2:B:311:EDO:H22	1.81	0.61
1:A:76:VAL:HG23	1:A:81:ILE:HG22	1.83	0.60
1:D:38:LYS:NZ	5:D:406:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLN:NE2	1:B:136:HIS:HB2	2.17	0.59
1:B:-1:ALA:N	5:B:401:HOH:O	2.17	0.58
1:D:61:ARG:HD3	1:D:63:LYS:HZ1	1.68	0.57
1:D:135:ARG:NH1	1:D:156:ASP:OD1	2.29	0.56
1:B:184:LYS:HD3	1:B:202:GLU:OE1	2.06	0.56
1:D:241:VAL:HG12	1:D:269:LEU:HD21	1.87	0.56
1:A:37:TYR:HE2	1:A:76:VAL:HG12	1.69	0.56
1:D:24:ASP:OD1	1:D:57:ARG:HD3	2.05	0.56
1:B:214:LYS:HD2	1:B:249:TYR:CZ	2.41	0.55
1:B:120:LYS:NZ	5:B:409:HOH:O	2.38	0.55
1:C:61:ARG:HH22	2:C:301:EDO:H21	1.71	0.55
1:A:5:ILE:HG23	1:A:6:LYS:H	1.74	0.53
1:B:228:ARG:HD3	5:B:613:HOH:O	2.08	0.53
1:C:178:GLU:OE2	5:C:403:HOH:O	2.19	0.53
1:C:108:CYS:HB3	1:C:149:ILE:HB	1.92	0.52
1:B:131:LYS:CG	1:B:133:GLN:HB3	2.40	0.52
1:B:131:LYS:HG2	1:B:133:GLN:OE1	2.10	0.52
1:D:22:GLU:OE1	1:D:57:ARG:HD2	2.10	0.51
1:D:141:GLU:OE1	1:D:146:LYS:NZ	2.33	0.51
1:C:131:LYS:H	1:C:131:LYS:CD	2.22	0.51
1:D:4:LEU:HA	1:D:25:ILE:HD12	1.92	0.51
1:C:101:THR:O	1:C:102:LEU:HD23	2.11	0.49
1:C:101:THR:HA	1:C:174:ARG:O	2.12	0.49
1:C:130:LEU:HD12	5:C:462:HOH:O	2.11	0.49
1:D:131:LYS:O	1:D:133:GLN:N	2.41	0.49
1:C:127:GLY:O	1:D:68:LYS:HE2	2.14	0.47
1:C:214:LYS:HD2	1:C:249:TYR:CZ	2.49	0.47
1:B:172:GLU:OE2	5:B:403:HOH:O	2.20	0.47
1:B:42:LYS:NZ	5:B:414:HOH:O	2.45	0.47
1:D:47:ASP:OD1	1:D:47:ASP:N	2.47	0.46
1:C:163:LYS:NZ	1:C:165:GLU:O	2.29	0.46
1:C:128:ARG:NH2	3:C:303:SO4:O1	2.43	0.46
2:C:302:EDO:H21	5:C:407:HOH:O	2.15	0.46
1:D:221:GLU:OE2	1:D:226:ASN:HA	2.15	0.45
1:D:212:TRP:NE1	5:D:407:HOH:O	2.36	0.45
1:D:23:ILE:HG23	1:D:58:HIS:HB2	1.99	0.45
1:D:61:ARG:HD3	1:D:63:LYS:HZ2	1.78	0.45
1:A:127:GLY:O	1:B:68:LYS:HE2	2.17	0.45
1:B:133:GLN:HE21	1:B:136:HIS:HB2	1.81	0.45
1:B:165:GLU:HB3	1:B:166:ASP:H	1.59	0.45
1:C:250:SER:OG	1:C:264:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LYS:HE3	1:C:120:LYS:HB2	1.41	0.44
1:D:2:VAL:HB	1:D:25:ILE:HD11	2.00	0.44
1:D:131:LYS:C	1:D:133:GLN:N	2.72	0.43
1:B:31:GLU:H	1:B:31:GLU:CD	2.19	0.43
1:A:5:ILE:CG2	1:A:24:ASP:HB3	2.48	0.43
1:B:131:LYS:HG2	1:B:133:GLN:HB3	2.01	0.43
1:D:3:THR:HB	1:D:26:LYS:HB2	2.01	0.43
1:C:31:GLU:H	1:C:31:GLU:CD	2.19	0.42
1:A:50:GLU:HB2	1:A:61:ARG:HB3	2.00	0.42
1:D:188:ASN:O	1:D:189:ILE:HD13	2.19	0.42
1:D:190:VAL:HG12	1:D:268:TYR:HB2	2.01	0.42
1:C:131:LYS:HE2	5:C:408:HOH:O	2.19	0.42
1:D:195:GLN:HG3	5:D:454:HOH:O	2.19	0.42
1:A:190:VAL:HG22	1:A:268:TYR:HB2	2.01	0.42
1:C:262:ARG:HE	1:C:264:THR:CG2	2.32	0.42
1:A:18:ASP:OD1	1:A:63:LYS:HD3	2.20	0.41
1:C:125:ARG:NH2	1:C:155:GLU:O	2.53	0.41
1:A:185:ARG:NH1	5:A:417:HOH:O	2.48	0.41
1:A:224:LYS:NZ	5:A:415:HOH:O	2.53	0.41
1:C:50:GLU:HB2	1:C:61:ARG:HB3	2.01	0.41
1:B:186:ILE:HG23	1:B:201:CYS:HB3	2.03	0.41
1:D:186:ILE:HG23	1:D:201:CYS:HB3	2.02	0.41
1:D:186:ILE:HG12	1:D:263:SER:OG	2.20	0.41
1:B:108:CYS:HB2	1:B:152:VAL:HG11	2.02	0.40
1:B:241:VAL:HG12	1:B:269:LEU:HD21	2.04	0.40
1:D:245:ASP:O	1:D:267:LEU:HD23	2.22	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-1:ALA:C	2:C:305:EDO:O2[4_555]	1.37	0.83
1:D:-1:ALA:CA	2:C:305:EDO:O2[4_555]	1.68	0.52
1:D:-1:ALA:O	2:C:305:EDO:O2[4_555]	1.84	0.36
5:B:544:HOH:O	5:C:544:HOH:O[3_655]	2.10	0.10
5:A:556:HOH:O	5:C:559:HOH:O[1_465]	2.12	0.08
5:C:512:HOH:O	5:D:453:HOH:O[1_545]	2.14	0.06
5:B:644:HOH:O	5:D:440:HOH:O[4_465]	2.16	0.04
5:A:629:HOH:O	5:B:577:HOH:O[3_745]	2.17	0.03

## 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	270/273 (99%)	263 (97%)	7 (3%)	0	100	100
1	B	270/273 (99%)	264 (98%)	5 (2%)	1 (0%)	34	24
1	C	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
1	D	271/273 (99%)	262 (97%)	8 (3%)	1 (0%)	34	24
All	All	1080/1092 (99%)	1053 (98%)	25 (2%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	134	GLY
1	B	134	GLY

### 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	246/246 (100%)	243 (99%)	3 (1%)	71	70
1	B	246/246 (100%)	244 (99%)	2 (1%)	81	82
1	C	245/246 (100%)	244 (100%)	1 (0%)	91	91
1	D	247/246 (100%)	244 (99%)	3 (1%)	71	70
All	All	984/984 (100%)	975 (99%)	9 (1%)	78	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	24	ASP
1	A	26	LYS
1	B	153	ARG
1	B	184	LYS
1	C	131	LYS
1	D	185	ARG
1	D	235	TYR
1	D	262	ARG

Sometimes 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](#)

30 ligands are modelled in this entry.

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	SO4	B	304	-	4,4,4	0.13	0	6,6,6	0.15	0
2	EDO	B	301	-	3,3,3	0.51	0	2,2,2	0.25	0
2	EDO	D	306	-	3,3,3	0.50	0	2,2,2	0.18	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	D	305	-	3,3,3	0.60	0	2,2,2	0.10	0
2	EDO	B	309	-	3,3,3	0.49	0	2,2,2	0.25	0
3	SO4	B	308	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.10	0
2	EDO	B	310	-	3,3,3	0.59	0	2,2,2	0.05	0
3	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.16	0
2	EDO	A	303	-	3,3,3	0.61	0	2,2,2	0.15	0
2	EDO	A	304	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	C	305	-	3,3,3	0.55	0	2,2,2	0.12	0
4	GOL	C	306	-	5,5,5	1.09	1 (20%)	5,5,5	1.10	0
2	EDO	B	312	-	3,3,3	0.46	0	2,2,2	0.50	0
2	EDO	C	301	-	3,3,3	0.40	0	2,2,2	0.57	0
2	EDO	C	302	-	3,3,3	0.43	0	2,2,2	0.57	0
2	EDO	B	311	-	3,3,3	0.42	0	2,2,2	0.45	0
2	EDO	A	305	-	3,3,3	0.52	0	2,2,2	0.26	0
2	EDO	A	301	-	3,3,3	0.44	0	2,2,2	0.38	0
3	SO4	B	306	-	4,4,4	0.11	0	6,6,6	0.47	0
3	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.08	0
2	EDO	B	313	-	3,3,3	0.49	0	2,2,2	0.33	0
2	EDO	D	304	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	B	302	-	3,3,3	0.58	0	2,2,2	0.01	0
3	SO4	B	305	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	B	307	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	D	303	-	4,4,4	0.15	0	6,6,6	0.08	0
2	EDO	D	301	-	3,3,3	0.60	0	2,2,2	0.36	0
2	EDO	A	302	-	3,3,3	0.40	0	2,2,2	0.59	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
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	D	306	-	-	1/1/1/1	-
2	EDO	D	305	-	-	1/1/1/1	-
2	EDO	B	309	-	-	1/1/1/1	-
2	EDO	B	310	-	-	1/1/1/1	-
2	EDO	A	303	-	-	0/1/1/1	-
2	EDO	A	304	-	-	0/1/1/1	-
2	EDO	C	305	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	306	-	-	2/4/4/4	-
2	EDO	B	312	-	-	1/1/1/1	-
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	C	302	-	-	0/1/1/1	-
2	EDO	B	311	-	-	0/1/1/1	-
2	EDO	A	305	-	-	0/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	B	313	-	-	0/1/1/1	-
2	EDO	D	304	-	-	0/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	D	301	-	-	1/1/1/1	-
2	EDO	A	302	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	306	GOL	C1-C2	2.20	1.60	1.51

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	GOL	C1-C2-C3-O3
4	C	306	GOL	O2-C2-C3-O3
2	A	301	EDO	O1-C1-C2-O2
2	B	310	EDO	O1-C1-C2-O2
2	D	301	EDO	O1-C1-C2-O2
2	D	305	EDO	O1-C1-C2-O2
2	B	309	EDO	O1-C1-C2-O2
2	B	312	EDO	O1-C1-C2-O2
2	D	306	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	305	EDO	0	3
2	C	301	EDO	1	0
2	C	302	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	311	EDO	1	0
3	C	303	SO4	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	271/273 (99%)	-0.29	3 (1%) 80 82	24, 42, 76, 96	1 (0%)
1	B	272/273 (99%)	-0.30	2 (0%) 87 89	26, 39, 66, 119	0
1	C	271/273 (99%)	-0.21	1 (0%) 92 93	25, 43, 82, 102	0
1	D	272/273 (99%)	0.26	14 (5%) 28 30	30, 64, 106, 138	1 (0%)
All	All	1086/1092 (99%)	-0.14	20 (1%) 68 71	24, 45, 90, 138	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	ALA	6.1
1	D	238	ILE	3.6
1	D	198	THR	2.9
1	B	134	GLY	2.9
1	D	228	ARG	2.9
1	D	189	ILE	2.9
1	D	241	VAL	2.7
1	D	229	ASN	2.7
1	D	32	ILE	2.6
1	D	190	VAL	2.5
1	D	236	MET	2.5
1	D	268	TYR	2.3
1	A	29	TYR	2.3
1	D	196	SER	2.3
1	B	132	PRO	2.3
1	A	4	LEU	2.2
1	D	214	LYS	2.2
1	D	33	LYS	2.2
1	C	128	ARG	2.1
1	A	81	ILE	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 [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	310	4/4	0.50	0.31	70,71,72,73	0
2	EDO	B	313	4/4	0.59	0.22	73,75,76,78	0
2	EDO	A	303	4/4	0.63	0.25	46,55,66,68	0
2	EDO	D	306	4/4	0.67	0.50	75,83,88,89	0
2	EDO	D	305	4/4	0.79	0.27	49,52,63,65	0
2	EDO	D	304	4/4	0.79	0.24	70,73,80,80	0
3	SO4	B	308	5/5	0.79	0.24	133,135,140,142	0
2	EDO	B	311	4/4	0.81	0.47	77,78,79,80	0
2	EDO	C	302	4/4	0.81	0.16	69,69,73,85	0
2	EDO	C	305	4/4	0.84	0.43	76,95,107,112	0
2	EDO	D	301	4/4	0.84	0.17	36,42,62,62	0
2	EDO	B	302	4/4	0.84	0.21	60,70,76,78	0
3	SO4	C	304	5/5	0.84	0.19	119,121,122,124	0
3	SO4	D	302	5/5	0.86	0.19	105,110,112,119	0
4	GOL	C	306	6/6	0.87	0.13	48,55,55,64	0
2	EDO	B	312	4/4	0.88	0.11	64,67,73,75	0
2	EDO	A	301	4/4	0.88	0.12	59,60,66,66	0
3	SO4	D	303	5/5	0.89	0.20	128,130,132,135	0
2	EDO	A	305	4/4	0.90	0.14	49,49,51,60	0
2	EDO	C	301	4/4	0.91	0.16	51,57,58,66	0
2	EDO	B	301	4/4	0.91	0.20	45,52,53,55	0
2	EDO	A	302	4/4	0.91	0.12	52,53,66,77	0
2	EDO	A	304	4/4	0.92	0.19	63,64,71,77	0
3	SO4	B	307	5/5	0.93	0.26	156,159,161,163	0
2	EDO	B	309	4/4	0.93	0.11	45,46,47,54	0
3	SO4	B	305	5/5	0.95	0.11	92,98,101,103	0
3	SO4	C	303	5/5	0.95	0.11	100,100,105,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	304	5/5	0.95	0.14	107,110,114,115	0
3	SO4	B	306	5/5	0.98	0.10	41,45,54,61	0
3	SO4	B	303	5/5	0.98	0.11	66,67,73,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.