



# Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 01:33 PM BST

PDB ID : 4NXT  
Title : Crystal structure of the cytosolic domain of human MiD51  
Authors : Richter, V.; Ryan, M.T.; Kvansakul, M.  
Deposited on : 2013-12-09  
Resolution : 2.12 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

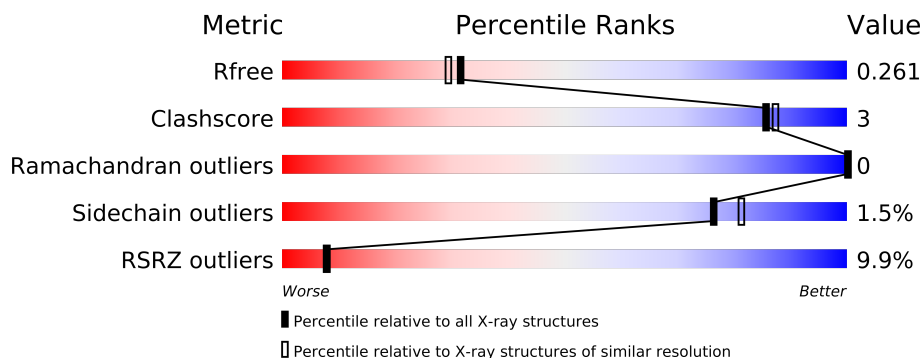
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23004  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 2.12 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))
$R_{free}$	66092	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	B	501	-	X
2	GOL	C	501	-	X
2	GOL	C	503	-	X
2	GOL	C	504	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	502	-	X
3	SO4	C	506	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21243 atoms, of which 10351 are hydrogens and 0 are deuterium.

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 Mitochondrial dynamic protein MID51.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	H	N	O	S	0	1	0
			5217	1676	2606	444	479	12			
1	B	331	Total	C	H	N	O	S	0	2	0
			5162	1661	2581	430	478	12			
1	C	331	Total	C	H	N	O	S	0	0	0
			5176	1658	2594	438	474	12			
1	D	326	Total	C	H	N	O	S	0	0	0
			5007	1615	2491	424	466	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
A	118	SER	-	EXPRESSION TAG	UNP Q9NQG6
B	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
B	118	SER	-	EXPRESSION TAG	UNP Q9NQG6
C	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
C	118	SER	-	EXPRESSION TAG	UNP Q9NQG6
D	117	GLY	-	EXPRESSION TAG	UNP Q9NQG6
D	118	SER	-	EXPRESSION TAG	UNP Q9NQG6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			13	3	7	3		

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



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

- Molecule 4 is water.

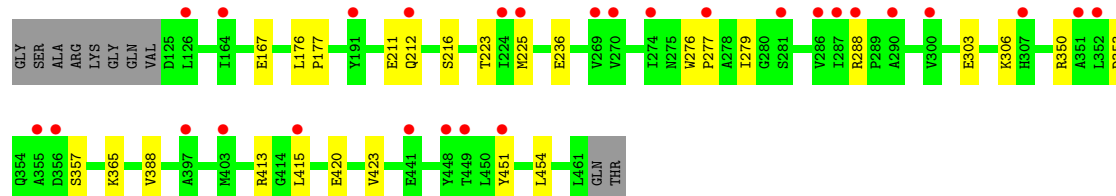
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	158	Total	O	0	0
			158	158		
4	C	124	Total	O	0	0
			124	124		
4	D	88	Total	O	0	0
			88	88		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

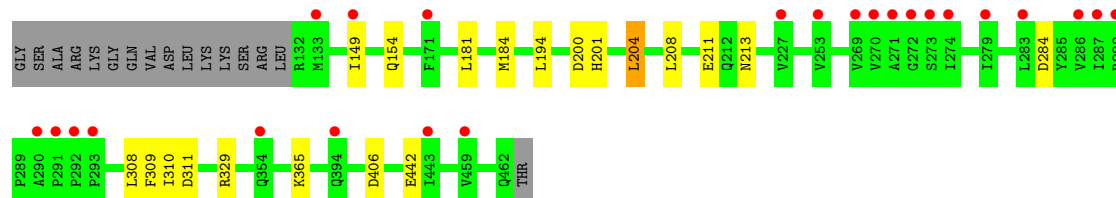
- Molecule 1: Mitochondrial dynamic protein MID51

Chain A: 



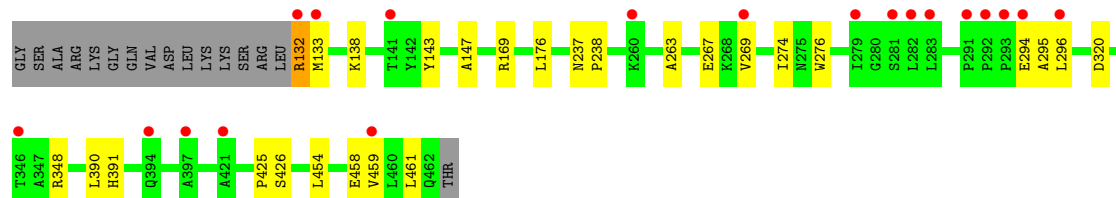
- Molecule 1: Mitochondrial dynamic protein MID51

Chain B: 



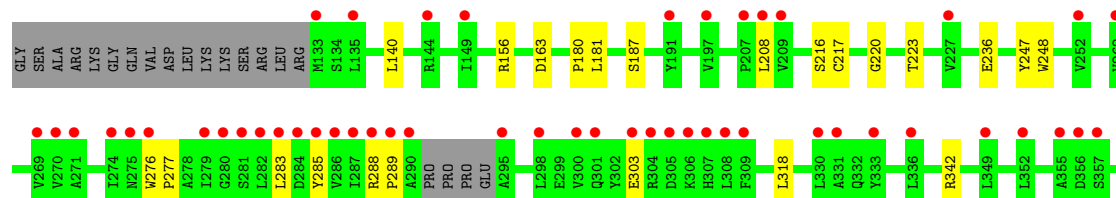
- Molecule 1: Mitochondrial dynamic protein MID51

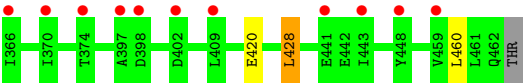
Chain C: 



- Molecule 1: Mitochondrial dynamic protein MID51

Chain D: 







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.72Å 78.73Å 79.36Å 66.26° 84.93° 64.07°	Depositor
Resolution (Å)	39.01 – 2.12 39.01 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.3 (39.01-2.12) 97.3 (39.01-2.12)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.223 , 0.263 0.222 , 0.261	Depositor DCC
$R_{free}$ test set	3961 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 79557 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.24	0/2673	0.42	0/3648
1	B	0.25	0/2646	0.43	0/3616
1	C	0.23	0/2641	0.44	0/3604
1	D	0.24	0/2571	0.43	0/3510
All	All	0.24	0/10531	0.43	0/14378

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2611	2606	0	13	0
1	B	2581	2581	0	12	1
1	C	2582	2594	0	14	0
1	D	2516	2491	0	16	0
2	A	6	8	0	0	0
2	B	6	8	0	0	0
2	C	24	32	0	2	1
2	D	24	31	1	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	C	10	0	0	1	0
4	A	157	0	0	3	0
4	B	158	0	0	0	0
4	C	124	0	0	1	0
4	D	88	0	0	0	0
All	All	10892	10351	1	56	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (56) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:200:ASP:OD1	1:B:201:HIS:ND1	2.17	0.78
1:C:294:GLU:CB	1:C:295:ALA:HA	2.19	0.73
1:D:156:ARG:NH1	1:D:303:GLU:OE2	2.23	0.72
1:D:220:GLY:O	1:D:223:THR:OG1	2.11	0.68
1:A:413:ARG:NH2	4:A:721:HOH:O	2.28	0.66
1:C:459:VAL:O	4:C:656:HOH:O	2.15	0.64
1:C:132:ARG:HE	1:C:132:ARG:HA	1.61	0.64
1:B:211:GLU:OE1	1:B:213:ASN:N	2.33	0.61
1:A:451:TYR:CD1	1:A:454:LEU:HD11	2.39	0.58
1:C:169:ARG:NH2	3:C:505:SO4:O3	2.35	0.57
1:D:180:PRO:HG3	1:D:247:TYR:HB3	1.85	0.57
1:A:211:GLU:OE2	4:A:745:HOH:O	2.18	0.56
1:D:276:TRP:N	1:D:277:PRO:HD2	2.22	0.55
1:A:167:GLU:HG2	1:A:279:ILE:HG23	1.91	0.53
1:D:288:ARG:HD2	1:D:289:PRO:HD2	1.91	0.52
1:D:318:LEU:HD23	2:D:501:GOL:H11	1.92	0.51
1:B:184:MET:HB3	1:B:204:LEU:CD2	2.41	0.51
1:B:329:ARG:NH2	1:B:442:GLU:OE1	2.44	0.51
1:A:420:GLU:OE2	1:A:451:TYR:OH	2.28	0.49
1:A:212:GLN:NE2	3:A:502:SO4:O4	2.44	0.48
1:D:217:CYS:HB3	1:D:318:LEU:HD12	1.95	0.47
1:C:237:ASN:N	1:C:238:PRO:HD3	2.29	0.47
2:C:501:GOL:O3	2:C:501:GOL:O1	2.30	0.47
1:D:163:ASP:HB3	1:D:283:LEU:HD22	1.97	0.47
1:B:194:LEU:HA	1:B:365:LYS:HE3	1.97	0.47
1:A:216:SER:OG	1:A:236:GLU:OE2	2.32	0.46
1:C:263:ALA:HB1	1:C:296:LEU:HD11	1.98	0.46
1:C:348:ARG:HD3	1:C:390:LEU:HD22	1.99	0.45
1:B:149[B]:ILE:HD12	1:B:154:GLN:HB2	1.99	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:181:LEU:HD23	1:D:208:LEU:HA	2.00	0.44
1:A:365:LYS:NZ	4:A:748:HOH:O	2.51	0.43
1:C:138:LYS:HG2	1:C:461:LEU:HD12	1.99	0.43
2:C:504:GOL:H32	1:D:420:GLU:HB3	2.00	0.43
1:C:143:TYR:HA	1:C:147:ALA:HB3	2.00	0.43
1:B:181:LEU:HD23	1:B:208:LEU:HA	2.01	0.43
1:B:308:LEU:HD21	1:B:310:ILE:HG13	2.01	0.42
1:B:308:LEU:HD22	1:B:309:PHE:N	2.33	0.42
1:D:208:LEU:HG	1:D:248:TRP:CZ2	2.55	0.42
1:A:303:GLU:CG	1:A:306:LYS:HB2	2.50	0.42
1:D:180:PRO:HG3	1:D:247:TYR:CB	2.49	0.42
1:B:204:LEU:HD12	1:B:310:ILE:HG21	2.02	0.42
1:D:216:SER:OG	1:D:236:GLU:OE2	2.34	0.41
1:D:187:SER:OG	1:D:342:ARG:NH2	2.51	0.41
1:C:391:HIS:NE2	1:C:425:PRO:O	2.54	0.41
1:B:308:LEU:CD2	1:B:310:ILE:CG1	2.98	0.41
1:C:274:ILE:HD13	1:C:276:TRP:CZ2	2.56	0.41
1:A:388:VAL:HG21	1:A:415:LEU:HD12	2.02	0.41
1:A:276:TRP:HB2	1:A:277:PRO:HD3	2.01	0.41
1:D:283:LEU:HB3	1:D:285:TYR:CD2	2.55	0.41
1:C:176:LEU:HD13	1:C:269:VAL:HG12	2.02	0.41
1:C:132:ARG:HE	1:C:132:ARG:CA	2.31	0.41
1:D:428:LEU:HD23	1:D:428:LEU:N	2.35	0.41
1:B:308:LEU:HD22	1:B:308:LEU:C	2.41	0.40
1:C:267:GLU:HB2	1:C:296:LEU:HD21	2.03	0.40
1:A:353:ASP:O	1:A:357:SER:N	2.54	0.40
1:A:176:LEU:N	1:A:177:PRO:CD	2.85	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:406:ASP:OD2	2:C:501:GOL:O3[1_554]	2.13	0.07

## 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	336/347 (97%)	327 (97%)	9 (3%)	0	100	100
1	B	331/347 (95%)	325 (98%)	6 (2%)	0	100	100
1	C	329/347 (95%)	320 (97%)	9 (3%)	0	100	100
1	D	322/347 (93%)	307 (95%)	15 (5%)	0	100	100
All	All	1318/1388 (95%)	1279 (97%)	39 (3%)	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	279/298 (94%)	274 (98%)	5 (2%)	71	75
1	B	279/298 (94%)	276 (99%)	3 (1%)	84	88
1	C	279/298 (94%)	273 (98%)	6 (2%)	64	68
1	D	267/298 (90%)	264 (99%)	3 (1%)	84	88
All	All	1104/1192 (93%)	1087 (98%)	17 (2%)	76	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	THR
1	A	225	MET
1	A	288	ARG
1	A	350	ARG
1	A	423	VAL
1	B	204	LEU
1	B	284	ASP
1	B	311	ASP
1	C	132	ARG
1	C	133	MET
1	C	320	ASP
1	C	426	SER
1	C	454	LEU
1	C	458	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	140	LEU
1	D	428	LEU
1	D	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	203	GLN
1	A	212	GLN
1	A	387	ASN
1	B	154	GLN
1	C	159	GLN
1	C	387	ASN
1	D	203	GLN
1	D	226	ASN
1	D	387	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 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	$\# Z  > 2$
2	GOL	A	501	-	5,5,5	0.35	0	5,5,5	0.25	0
3	SO4	A	502	-	4,4,4	0.21	0	6,6,6	0.09	0
2	GOL	B	501	-	5,5,5	0.36	0	5,5,5	0.20	0
2	GOL	C	501	-	5,5,5	0.35	0	5,5,5	0.36	0
2	GOL	C	502	-	5,5,5	0.44	0	5,5,5	0.10	0
2	GOL	C	503	-	5,5,5	0.33	0	5,5,5	0.27	0
2	GOL	C	504	-	5,5,5	0.39	0	5,5,5	0.23	0
3	SO4	C	505	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	C	506	-	4,4,4	0.19	0	6,6,6	0.08	0
2	GOL	D	501	-	5,5,5	0.31	0	5,5,5	0.40	0
2	GOL	D	502	-	5,5,5	0.35	0	5,5,5	0.21	0
2	GOL	D	503	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	D	504	-	5,5,5	0.35	0	5,5,5	0.49	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	GOL	A	501	-	-	0/4/4/4	0/0/0/0
3	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	502	-	-	0/4/4/4	0/0/0/0
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
2	GOL	C	504	-	-	0/4/4/4	0/0/0/0
3	SO4	C	505	-	-	0/0/0/0	0/0/0/0
3	SO4	C	506	-	-	0/0/0/0	0/0/0/0
2	GOL	D	501	-	-	0/4/4/4	0/0/0/0
2	GOL	D	502	-	-	0/4/4/4	0/0/0/0
2	GOL	D	503	-	-	0/4/4/4	0/0/0/0
2	GOL	D	504	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	337/347 (97%)	0.64	28 (8%)	11 12	23, 45, 74, 104	0
1	B	331/347 (95%)	0.68	24 (7%)	15 16	24, 41, 69, 108	0
1	C	331/347 (95%)	0.57	19 (5%)	23 25	23, 40, 69, 121	0
1	D	326/347 (93%)	1.12	61 (18%)	2 2	34, 59, 96, 122	0
All	All	1325/1388 (95%)	0.75	132 (9%)	8 8	23, 46, 83, 122	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	283	LEU	8.7
1	D	355	ALA	8.1
1	D	287	ILE	7.6
1	A	355	ALA	7.2
1	D	305	ASP	6.4
1	B	270	VAL	6.2
1	D	286	VAL	6.1
1	D	279	ILE	5.8
1	D	397	ALA	5.7
1	B	293	PRO	5.6
1	B	291	PRO	5.5
1	D	300	VAL	5.5
1	B	272	GLY	5.4
1	D	282	LEU	4.9
1	B	286	VAL	4.5
1	B	290	ALA	4.4
1	D	290	ALA	4.3
1	A	397	ALA	4.2
1	D	307	HIS	4.1
1	D	274	ILE	4.0
1	A	300	VAL	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	290	ALA	3.9
1	D	295	ALA	3.7
1	D	280	GLY	3.7
1	B	279	ILE	3.7
1	C	132	ARG	3.6
1	A	274	ILE	3.6
1	D	448	TYR	3.6
1	A	286	VAL	3.6
1	B	253	VAL	3.6
1	B	274	ILE	3.5
1	C	279	ILE	3.5
1	D	330	LEU	3.5
1	D	197	VAL	3.4
1	B	287	ILE	3.4
1	C	141	THR	3.3
1	D	275	ASN	3.2
1	A	270	VAL	3.2
1	D	149	ILE	3.2
1	A	281	SER	3.2
1	D	288	ARG	3.1
1	B	269	VAL	3.1
1	D	298	LEU	3.1
1	A	441	GLU	3.1
1	D	459	VAL	3.1
1	A	191	TYR	3.1
1	A	287	ILE	3.0
1	A	356	ASP	3.0
1	A	277	PRO	3.0
1	D	262	VAL	3.0
1	D	402	ASP	3.0
1	B	292	PRO	2.9
1	D	303	GLU	2.8
1	D	135	LEU	2.8
1	B	133	MET	2.8
1	D	276	TRP	2.8
1	D	333	TYR	2.8
1	B	171	PHE	2.7
1	B	354	GLN	2.7
1	B	273	SER	2.7
1	C	293	PRO	2.7
1	D	301	GLN	2.7
1	D	209	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	270	VAL	2.7
1	D	331	ALA	2.6
1	C	394	GLN	2.6
1	D	284	ASP	2.6
1	C	292	PRO	2.6
1	B	288	ARG	2.6
1	D	271	ALA	2.6
1	B	394	GLN	2.6
1	C	269	VAL	2.6
1	A	126	LEU	2.5
1	C	133	MET	2.5
1	B	227	VAL	2.5
1	D	349	LEU	2.5
1	B	459	VAL	2.5
1	D	252	VAL	2.5
1	C	346	THR	2.4
1	C	283	LEU	2.4
1	D	370	ILE	2.4
1	D	374	THR	2.4
1	A	224	ILE	2.4
1	D	304	ARG	2.4
1	D	366	ILE	2.4
1	B	271	ALA	2.4
1	D	309	PHE	2.4
1	A	352	LEU	2.3
1	A	449	THR	2.3
1	D	441	GLU	2.3
1	C	291	PRO	2.3
1	C	294	GLU	2.3
1	C	282	LEU	2.3
1	D	336	LEU	2.3
1	C	421	ALA	2.3
1	B	149[A]	ILE	2.3
1	D	289	PRO	2.3
1	D	306	LYS	2.3
1	D	144	ARG	2.2
1	A	415	LEU	2.2
1	C	397	ALA	2.2
1	D	227	VAL	2.2
1	A	164	ILE	2.2
1	A	403	MET	2.2
1	A	451	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	409	LEU	2.2
1	D	357	SER	2.2
1	B	283	LEU	2.1
1	D	308	LEU	2.1
1	B	443	ILE	2.1
1	D	443	ILE	2.1
1	D	398	ASP	2.1
1	C	459	VAL	2.1
1	D	285	TYR	2.1
1	D	281	SER	2.1
1	A	212	GLN	2.1
1	D	133	MET	2.1
1	D	207	PRO	2.1
1	D	356	ASP	2.1
1	D	269	VAL	2.1
1	C	281	SER	2.1
1	C	260	LYS	2.1
1	D	191	TYR	2.1
1	C	296	LEU	2.0
1	D	208	LEU	2.0
1	D	352	LEU	2.0
1	A	269	VAL	2.0
1	A	448	TYR	2.0
1	A	307	HIS	2.0
1	A	351	ALA	2.0
1	A	288	ARG	2.0
1	A	225	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	C	501	6/6	0.37	7.61	72,87,94,96	0
3	SO4	C	506	5/5	0.25	6.52	81,81,81,82	0
2	GOL	B	501	6/6	0.33	5.38	81,98,98,98	0
2	GOL	C	504	6/6	0.24	2.94	53,64,73,75	0
2	GOL	C	503	6/6	0.22	2.84	59,71,78,79	0
3	SO4	A	502	5/5	0.28	2.22	73,76,76,79	0
2	GOL	A	501	6/6	0.20	1.81	66,79,80,80	0
2	GOL	D	504	6/6	0.19	1.37	16,20,33,34	0
2	GOL	D	503	6/6	0.19	0.96	63,76,79,81	0
2	GOL	D	501	6/6	0.23	0.69	67,80,83,84	0
2	GOL	D	502	6/6	0.21	0.25	65,78,80,81	0
2	GOL	C	502	6/6	0.15	-0.18	62,74,77,77	0
3	SO4	C	505	5/5	0.12	-1.08	61,62,63,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.