



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:42 PM UTC

PDB ID : 4NXT / pdb_00004nxt
Title : Crystal structure of the cytosolic domain of human MiD51
Authors : Richter, V.; Ryan, M.T.; Kvensakul, M.
Deposited on : 2013-12-09
Resolution : 2.12 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

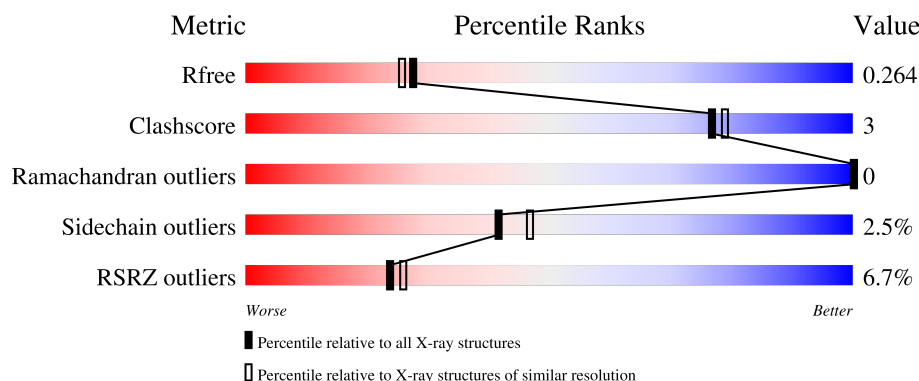
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 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	347	
1	B	347	
1	C	347	
1	D	347	

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 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 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:

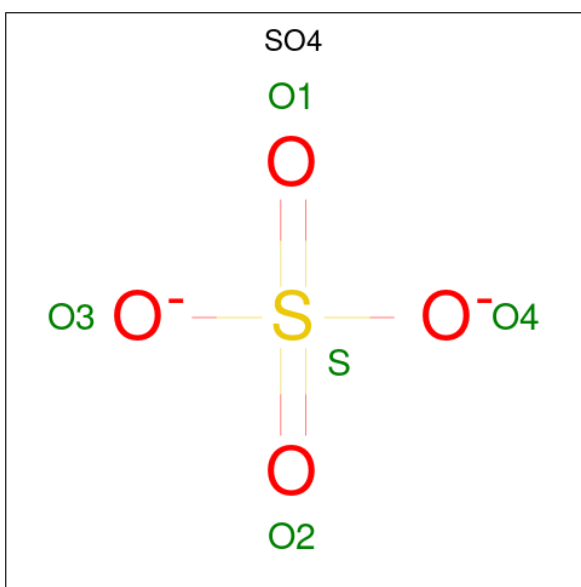
Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	expression tag	UNP Q9NQG6
A	118	SER	-	expression tag	UNP Q9NQG6
B	117	GLY	-	expression tag	UNP Q9NQG6
B	118	SER	-	expression tag	UNP Q9NQG6
C	117	GLY	-	expression tag	UNP Q9NQG6
C	118	SER	-	expression tag	UNP Q9NQG6
D	117	GLY	-	expression tag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

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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 (CCD ID: SO4) (formula: O₄S).



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		

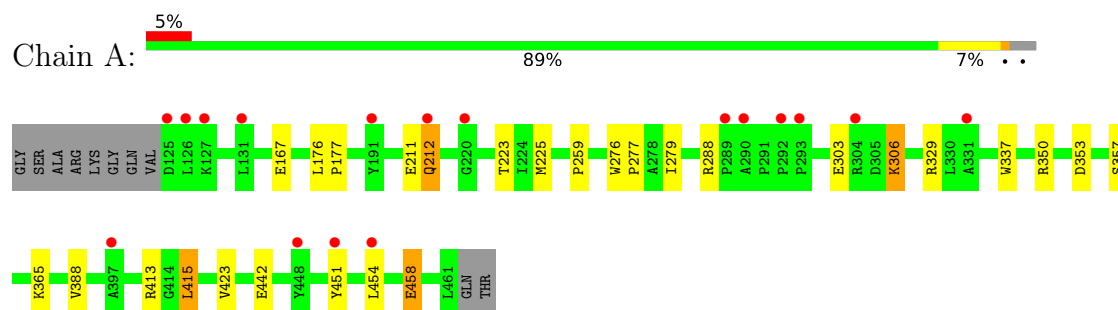
- Molecule 4 is water.

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		

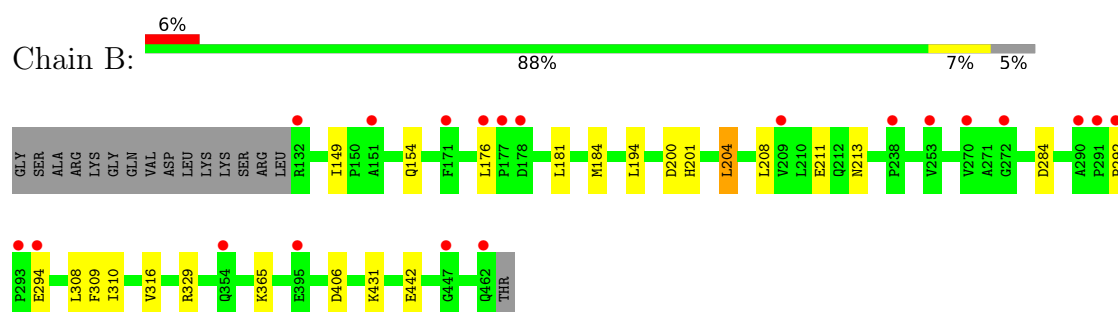
3 Residue-property plots [i](#)

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.

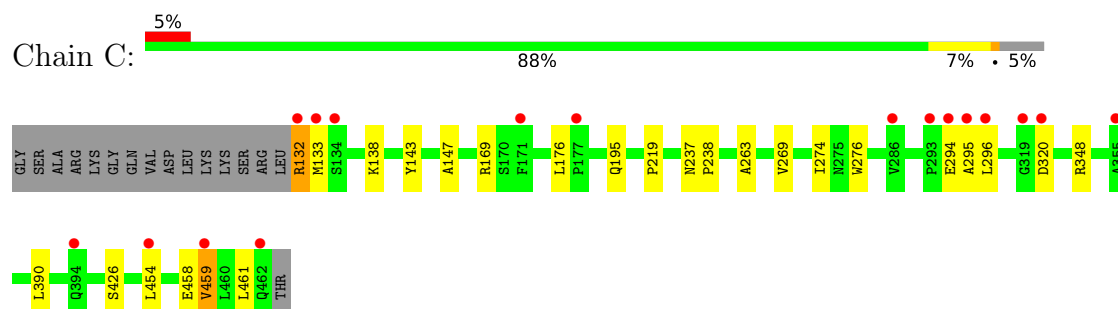
- Molecule 1: Mitochondrial dynamic protein MID51



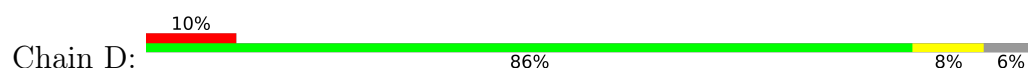
- Molecule 1: Mitochondrial dynamic protein MID51

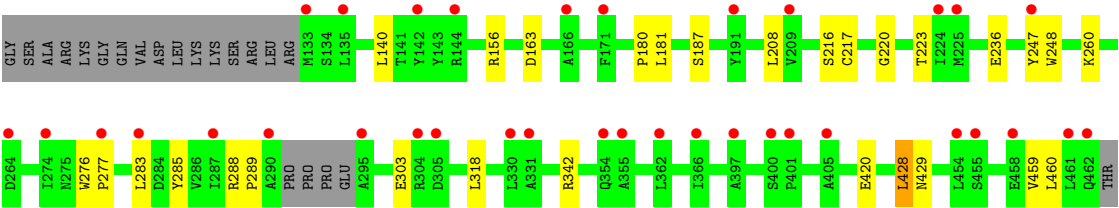


- Molecule 1: Mitochondrial dynamic protein MID51



- Molecule 1: Mitochondrial dynamic protein MID51





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.223 , 0.263 0.225 , 0.264	Depositor DCC
R_{free} test set	3964 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21243	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/2673	0.67	0/3648
1	B	0.34	0/2646	0.68	0/3616
1	C	0.32	0/2641	0.68	1/3604 (0.0%)
1	D	0.34	0/2571	0.67	0/3510
All	All	0.33	0/10531	0.67	1/14378 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	459	VAL	N-CA-C	-5.18	105.66	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2611	2606	2615	14	0
1	B	2581	2581	2587	15	1
1	C	2582	2594	2599	13	0
1	D	2516	2491	2498	17	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	32	32	3	1
2	D	24	31	32	1	0
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	10379	60	1

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 3.

All (60) 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:D:156:ARG:NH1	1:D:303:GLU:OE2	2.23	0.72
1:C:294:GLU:CB	1:C:295:ALA:HA	2.21	0.70
1:B:200:ASP:OD1	1:B:201:HIS:ND1	2.17	0.67
1:A:413:ARG:NH2	4:A:721:HOH:O	2.28	0.66
1:D:220:GLY:O	1:D:223:THR:OG1	2.11	0.66
1:C:459:VAL:O	4:C:656:HOH:O	2.15	0.64
1:C:132:ARG:HA	1:C:132:ARG:HE	1.61	0.64
1:B:211:GLU:OE1	1:B:213:ASN:N	2.33	0.61
1:D:180:PRO:HG3	1:D:247:TYR:HB3	1.82	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:A:211:GLU:OE2	4:A:745:HOH:O	2.18	0.56
1:A:167:GLU:HG2	1:A:279:ILE:HG23	1.89	0.55
1:D:276:TRP:N	1:D:277:PRO:HD2	2.23	0.54
1:B:184:MET:HB3	1:B:204:LEU:CD2	2.39	0.52
1:D:318:LEU:HD23	2:D:501:GOL:H11	1.91	0.52
1:B:329:ARG:NH2	1:B:442:GLU:OE1	2.44	0.51
1:B:194:LEU:HA	1:B:365:LYS:HE3	1.94	0.50
1:D:288:ARG:HD2	1:D:289:PRO:HD2	1.94	0.49
1:A:212:GLN:NE2	3:A:502:SO4:O4	2.44	0.48
1:C:348:ARG:HD3	1:C:390:LEU:HD22	1.97	0.47
1:D:163:ASP:HB3	1:D:283:LEU:HD22	1.96	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:B:292:PRO:HA	1:B:294:GLU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:CYS:HB3	1:D:318:LEU:HD12	1.96	0.46
1:C:263:ALA:HB1	1:C:296:LEU:HD11	1.98	0.46
1:B:149[B]:ILE:HD13	1:B:154:GLN:HB2	1.97	0.45
1:B:292:PRO:HA	1:B:294:GLU:N	2.32	0.45
1:D:181:LEU:HD23	1:D:208:LEU:HA	1.99	0.45
1:B:308:LEU:C	1:B:308:LEU:HD23	2.42	0.45
1:C:138:LYS:HG2	1:C:461:LEU:HD12	1.98	0.45
1:B:181:LEU:HD23	1:B:208:LEU:HA	1.99	0.45
2:C:504:GOL:H32	1:D:420:GLU:HB3	1.99	0.45
1:B:308:LEU:HD22	1:B:310:ILE:HG13	1.99	0.44
1:D:156:ARG:HH11	1:D:303:GLU:CD	2.24	0.44
1:A:365:LYS:NZ	4:A:748:HOH:O	2.51	0.43
1:D:180:PRO:HG3	1:D:247:TYR:CB	2.47	0.43
1:A:329:ARG:HH12	1:A:442:GLU:CD	2.27	0.43
1:A:458:GLU:H	1:A:458:GLU:CD	2.27	0.43
1:A:276:TRP:HB2	1:A:277:PRO:HD3	2.00	0.42
1:D:283:LEU:HB3	1:D:285:TYR:CD2	2.54	0.42
1:B:204:LEU:HD12	1:B:310:ILE:HG21	2.02	0.42
1:B:308:LEU:HD23	1:B:309:PHE:N	2.34	0.42
1:C:176:LEU:HD13	1:C:269:VAL:HG12	2.01	0.42
1:D:216:SER:OG	1:D:236:GLU:OE2	2.34	0.41
1:C:143:TYR:HA	1:C:147:ALA:HB3	2.02	0.41
1:D:187:SER:OG	1:D:342:ARG:NH2	2.51	0.41
1:A:303:GLU:CG	1:A:306:LYS:HB2	2.50	0.41
1:A:388:VAL:HG21	1:A:415:LEU:HD12	2.02	0.41
1:C:274:ILE:HD13	1:C:276:TRP:CZ2	2.56	0.41
1:B:308:LEU:CD2	1:B:310:ILE:CG1	2.98	0.41
1:D:208:LEU:HG	1:D:248:TRP:CZ2	2.56	0.41
1:C:219:PRO:HB3	2:C:502:GOL:H12	2.03	0.41
1:C:132:ARG:HE	1:C:132:ARG:CA	2.31	0.41
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
1:A:259:PRO:HG3	1:A:337:TRP:CD1	2.56	0.40
1:B:149[B]:ILE:HD11	1:B:154:GLN:N	2.36	0.40
1:D:428:LEU:N	1:D:428:LEU:HD23	2.36	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	Interatomic distance (Å)	Clash overlap (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%)	270 (97%)	9 (3%)	34	37
1	B	279/298 (94%)	274 (98%)	5 (2%)	51	59
1	C	279/298 (94%)	272 (98%)	7 (2%)	42	47
1	D	267/298 (90%)	261 (98%)	6 (2%)	45	52
All	All	1104/1192 (93%)	1077 (98%)	27 (2%)	42	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	223	THR

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Mol	Chain	Res	Type
1	A	225	MET
1	A	288	ARG
1	A	306	LYS
1	A	350	ARG
1	A	415	LEU
1	A	423	VAL
1	A	458	GLU
1	B	176	LEU
1	B	204	LEU
1	B	284	ASP
1	B	316	VAL
1	B	431	LYS
1	C	132	ARG
1	C	133	MET
1	C	195	GLN
1	C	320	ASP
1	C	426	SER
1	C	454	LEU
1	C	458	GLU
1	D	140	LEU
1	D	260	LYS
1	D	428	LEU
1	D	429	ASN
1	D	459	VAL
1	D	460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	203	GLN
1	B	379	HIS
1	D	159	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	501	-	5,5,5	0.38	0	5,5,5	0.40	0
2	GOL	D	503	-	5,5,5	0.36	0	5,5,5	0.28	0
3	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.09	0
2	GOL	C	503	-	5,5,5	0.37	0	5,5,5	0.23	0
2	GOL	B	501	-	5,5,5	0.39	0	5,5,5	0.27	0
3	SO4	C	505	-	4,4,4	0.23	0	6,6,6	0.09	0
2	GOL	D	504	-	5,5,5	0.43	0	5,5,5	0.42	0
2	GOL	A	501	-	5,5,5	0.39	0	5,5,5	0.28	0
3	SO4	C	506	-	4,4,4	0.23	0	6,6,6	0.08	0
2	GOL	C	502	-	5,5,5	0.46	0	5,5,5	0.19	0
2	GOL	C	504	-	5,5,5	0.42	0	5,5,5	0.14	0
2	GOL	D	501	-	5,5,5	0.34	0	5,5,5	0.51	0
2	GOL	D	502	-	5,5,5	0.39	0	5,5,5	0.23	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	C	501	-	-	2/4/4/4	-
2	GOL	D	503	-	-	1/4/4/4	-
2	GOL	C	503	-	-	2/4/4/4	-
2	GOL	B	501	-	-	0/4/4/4	-
2	GOL	D	504	-	-	3/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	502	-	-	0/4/4/4	-
2	GOL	C	504	-	-	3/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-
2	GOL	D	502	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	GOL	O1-C1-C2-O2
2	C	501	GOL	O1-C1-C2-C3
2	D	501	GOL	O1-C1-C2-O2
2	D	501	GOL	O1-C1-C2-C3
2	D	502	GOL	O1-C1-C2-C3
2	D	502	GOL	C1-C2-C3-O3
2	A	501	GOL	O1-C1-C2-C3
2	C	503	GOL	C1-C2-C3-O3
2	C	504	GOL	O1-C1-C2-C3
2	C	504	GOL	C1-C2-C3-O3
2	D	504	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-O2
2	C	504	GOL	O1-C1-C2-O2
2	D	502	GOL	O2-C2-C3-O3
2	D	502	GOL	O1-C1-C2-O2
2	C	503	GOL	O2-C2-C3-O3
2	D	503	GOL	O1-C1-C2-O2
2	D	504	GOL	O1-C1-C2-O2
2	D	504	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	GOL	1	1
3	A	502	SO4	1	0
3	C	505	SO4	1	0
2	C	502	GOL	1	0
2	C	504	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	GOL	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	337/347 (97%)	0.55	17 (5%)	34 37	26, 50, 81, 117	1 (0%)
1	B	331/347 (95%)	0.59	20 (6%)	27 30	21, 44, 75, 118	2 (0%)
1	C	331/347 (95%)	0.53	17 (5%)	33 36	25, 44, 75, 135	0
1	D	326/347 (93%)	1.03	35 (10%)	11 12	37, 64, 103, 132	0
All	All	1325/1388 (95%)	0.67	89 (6%)	24 26	21, 50, 91, 135	3 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	283	LEU	5.2
1	D	305	ASP	5.1
1	B	177	PRO	5.1
1	D	290	ALA	5.0
1	D	295	ALA	4.6
1	B	178	ASP	4.6
1	B	272	GLY	4.4
1	D	355	ALA	4.1
1	C	459	VAL	4.0
1	B	290	ALA	3.9
1	C	294	GLU	3.9
1	D	304	ARG	3.7
1	D	133	MET	3.7
1	D	461	LEU	3.6
1	D	454	LEU	3.6
1	D	224	ILE	3.5
1	A	454	LEU	3.5
1	D	462	GLN	3.5
1	A	126	LEU	3.4
1	A	451	TYR	3.4
1	C	295	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	125	ASP	3.4
1	A	293	PRO	3.4
1	C	171	PHE	3.2
1	A	212	GLN	3.1
1	A	191	TYR	3.1
1	D	135	LEU	3.1
1	D	397	ALA	3.0
1	D	400	SER	3.0
1	A	292	PRO	3.0
1	D	401	PRO	3.0
1	D	331	ALA	3.0
1	D	405	ALA	2.9
1	A	131	LEU	2.9
1	B	238	PRO	2.9
1	B	293	PRO	2.8
1	C	462	GLN	2.8
1	B	447	GLY	2.8
1	C	355	ALA	2.8
1	B	270	VAL	2.8
1	B	291	PRO	2.8
1	C	177	PRO	2.8
1	C	319	GLY	2.8
1	A	448	TYR	2.8
1	C	133	MET	2.7
1	D	247	TYR	2.7
1	C	320	ASP	2.7
1	D	274	ILE	2.7
1	D	354	GLN	2.6
1	A	127	LYS	2.5
1	A	331	ALA	2.5
1	B	209	VAL	2.5
1	B	253	VAL	2.4
1	A	304	ARG	2.4
1	A	397	ALA	2.4
1	B	354	GLN	2.4
1	B	176	LEU	2.3
1	D	362	LEU	2.3
1	A	220	GLY	2.3
1	D	225	MET	2.3
1	B	292	PRO	2.3
1	C	132	ARG	2.3
1	D	366	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	462	GLN	2.3
1	D	287	ILE	2.3
1	D	209	VAL	2.3
1	C	293	PRO	2.3
1	D	330	LEU	2.3
1	D	458	GLU	2.2
1	D	277	PRO	2.2
1	A	290	ALA	2.2
1	B	151	ALA	2.2
1	C	394	GLN	2.2
1	D	166	ALA	2.2
1	C	134	SER	2.2
1	A	289	PRO	2.1
1	D	264	ASP	2.2
1	C	454	LEU	2.1
1	D	144	ARG	2.1
1	B	294	GLU	2.1
1	D	171	PHE	2.1
1	B	132	ARG	2.1
1	D	455	SER	2.1
1	D	142	TYR	2.1
1	D	191	TYR	2.1
1	B	395	GLU	2.1
1	C	286	VAL	2.1
1	B	171	PHE	2.0
1	C	296	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	D	502	6/6	0.66	0.12	65,78,80,81	0
2	GOL	C	501	6/6	0.67	0.28	72,87,94,96	0
2	GOL	D	501	6/6	0.69	0.15	67,80,83,84	0
3	SO4	C	506	5/5	0.75	0.11	81,81,81,82	0
2	GOL	C	502	6/6	0.78	0.14	62,74,77,77	0
3	SO4	A	502	5/5	0.78	0.15	73,76,76,79	0
2	GOL	A	501	6/6	0.78	0.13	66,79,80,80	0
2	GOL	D	504	6/6	0.79	0.15	16,20,33,34	0
2	GOL	D	503	6/6	0.81	0.13	63,76,79,81	0
2	GOL	B	501	6/6	0.81	0.18	81,98,98,98	0
2	GOL	C	504	6/6	0.84	0.11	53,64,73,75	0
2	GOL	C	503	6/6	0.85	0.16	59,71,78,79	0
3	SO4	C	505	5/5	0.86	0.13	61,62,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.