



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 1O7N / pdb_00001o7n
Title : NAPHTHALENE 1,2-DIOXYGENASE, TERNARY COMPLEX WITH
DIOXYGEN AND INDOLE
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maswamy, S.
Deposited on : 2002-11-11
Resolution : 1.40 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

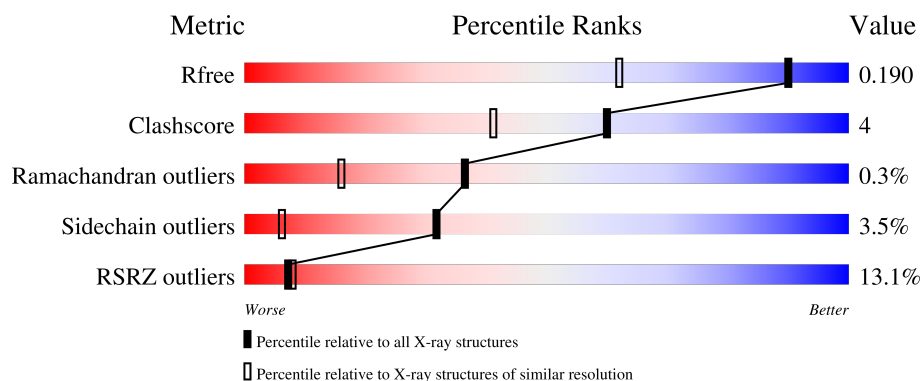
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	449	<div> <div>12%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
2	B	194	<div> <div>15%</div> <div>86%</div> <div>11%</div> <div>..</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
4	IND	A	505	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5699 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 NAPHTHALENE 1,2-DIOXYGENASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	1
			3481	2202	598	665	16			

- Molecule 2 is a protein called NAPHTHALENE 1,2-DIOXYGENASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1608	1007	302	293	6			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



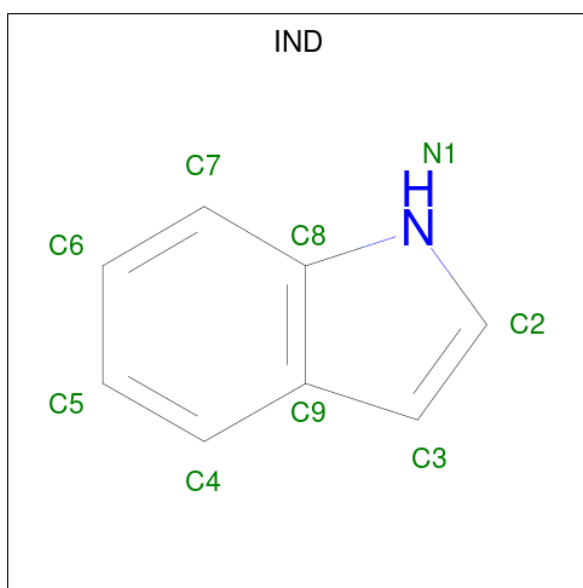
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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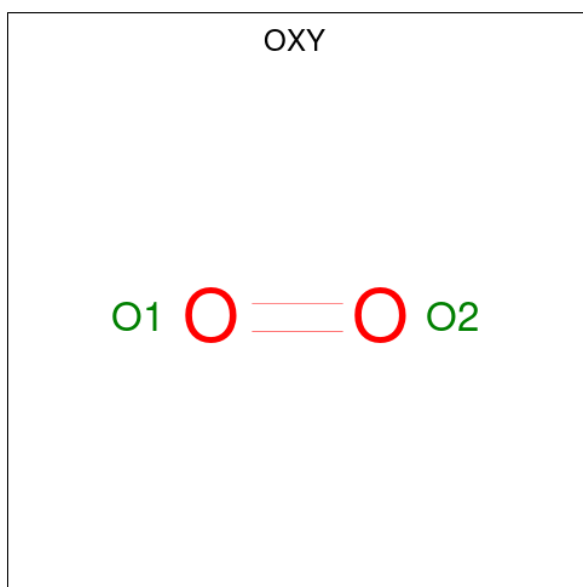
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is INDOLE (CCD ID: IND) (formula: C_8H_7N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	8	1		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



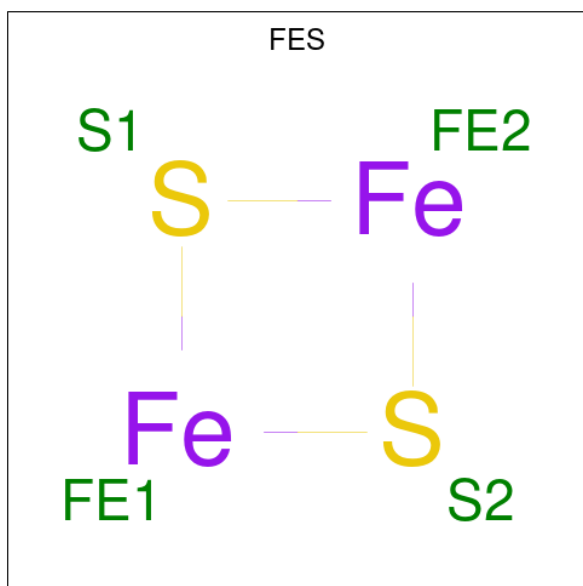
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Fe	0	0
			1	1		

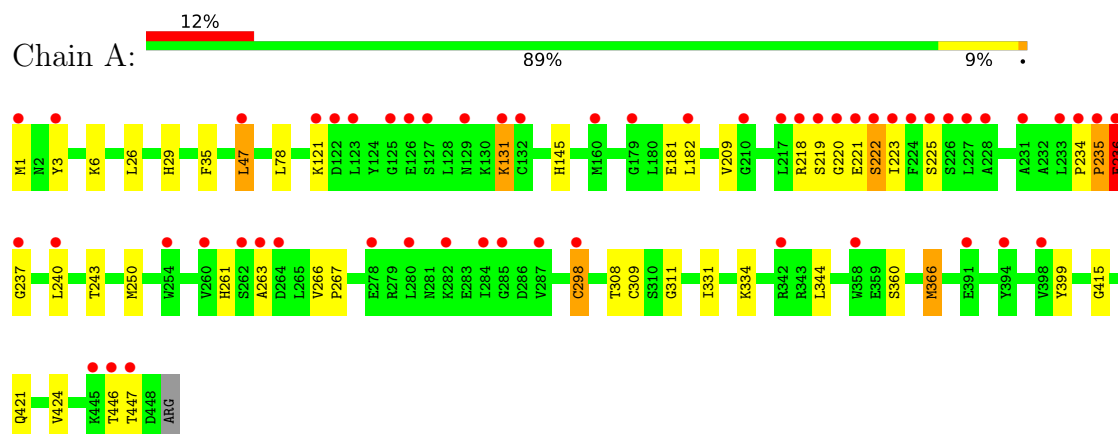
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	372	Total	O	0	0
			372	372		
9	B	174	Total	O	0	0
			174	174		

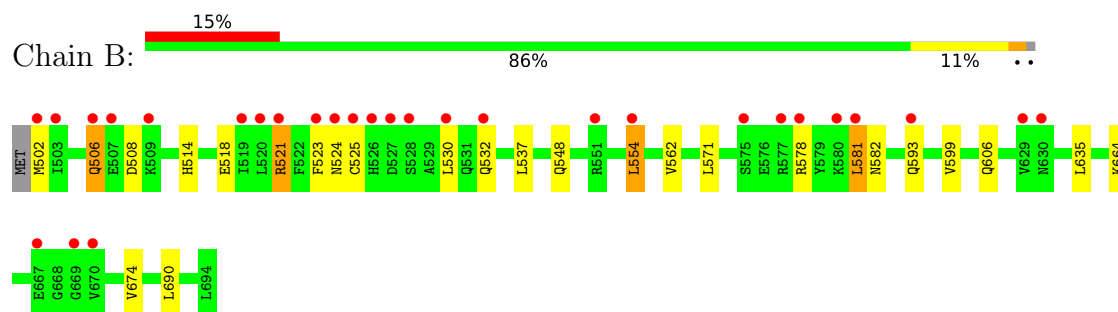
3 Residue-property plots [i](#)

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: NAPHTHALENE 1,2-DIOXYGENASE ALPHA SUBUNIT



• Molecule 2: NAPHTHALENE 1,2-DIOXYGENASE BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	139.83Å 139.83Å 208.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.40 40.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.00-1.40) 93.8 (40.00-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.0.36	Depositor
R, R_{free}	0.190 , 0.200 0.192 , 0.190	Depositor DCC
R_{free} test set	5901 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5699	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, SO4, EDO, FE, FES, IND

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	0.79	2/3573 (0.1%)	1.04	8/4841 (0.2%)
2	B	0.78	0/1638	0.99	3/2209 (0.1%)
All	All	0.79	2/5211 (0.0%)	1.03	11/7050 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	THR	C-N	-6.55	1.24	1.33
1	A	399	TYR	C-O	-5.37	1.20	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	548	GLN	OE1-CD-NE2	-9.34	113.27	122.60
1	A	421	GLN	OE1-CD-NE2	-9.08	113.52	122.60
1	A	145	HIS	CA-CB-CG	-7.86	105.94	113.80
1	A	222	SER	N-CA-C	6.95	121.19	110.42
2	B	548	GLN	CG-CD-NE2	6.24	125.75	116.40
1	A	421	GLN	CG-CD-NE2	6.09	125.54	116.40
1	A	366	MET	CA-CB-CG	5.82	125.75	114.10
2	B	562	VAL	N-CA-C	5.55	117.62	109.63
1	A	223	ILE	N-CA-C	5.49	117.91	111.05
1	A	209	VAL	N-CA-C	5.19	115.81	110.36
1	A	35	PHE	N-CA-C	5.12	117.76	111.82

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	3481	0	3316	28	0
2	B	1608	0	1583	16	0
3	A	20	0	30	1	0
3	B	8	0	12	0	0
4	A	9	0	7	0	0
5	A	2	0	0	0	0
6	A	5	0	0	1	0
6	B	15	0	0	0	0
7	A	4	0	0	0	0
8	A	1	0	0	0	0
9	A	372	0	0	2	0
9	B	174	0	0	6	0
All	All	5699	0	4948	43	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 4.

All (43) 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:A:250:MET:HB3	1:A:298:CYS:HB2	1.36	1.02
1:A:181:GLU:CG	1:A:334:LYS:HG2	2.00	0.90
1:A:181:GLU:HG3	1:A:334:LYS:HG2	1.57	0.84
1:A:250:MET:CB	1:A:298:CYS:HB2	2.08	0.81
1:A:181:GLU:HG3	1:A:334:LYS:CG	2.14	0.77
3:A:510:EDO:H21	2:B:581:LEU:HD13	1.66	0.77
2:B:523:PHE:HE1	9:B:854:HOH:O	1.75	0.67
2:B:523:PHE:CE1	9:B:854:HOH:O	2.48	0.66
1:A:3:TYR:CE2	1:A:26:LEU:HD13	2.35	0.61
2:B:537:LEU:HD12	9:B:947:HOH:O	2.00	0.60
2:B:525:CYS:SG	2:B:525:CYS:O	2.60	0.59
1:A:181:GLU:CG	1:A:334:LYS:CG	2.74	0.59
1:A:220:GLY:HA3	9:A:856:HOH:O	2.03	0.58
1:A:181:GLU:CD	1:A:334:LYS:HG2	2.31	0.55
1:A:221:GLU:O	1:A:263:ALA:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PRO:HB2	1:A:236:GLU:OE1	2.10	0.51
2:B:514:HIS:HD2	9:B:942:HOH:O	1.93	0.51
2:B:578:ARG:NH1	9:B:803:HOH:O	2.43	0.50
1:A:1:MET:SD	1:A:6:LYS:HG2	2.52	0.50
1:A:47:LEU:HD22	1:A:182:LEU:HD23	1.94	0.50
1:A:308:THR:O	1:A:309:CYS:HB2	2.12	0.49
1:A:181:GLU:HG3	1:A:334:LYS:HG3	1.93	0.48
2:B:506:GLN:HG3	9:B:830:HOH:O	2.14	0.47
2:B:530:LEU:HD21	2:B:635:LEU:CD1	2.45	0.47
1:A:311:GLY:HA2	1:A:331:ILE:HG13	1.97	0.47
1:A:236:GLU:HB2	1:A:237:GLY:H	1.38	0.46
1:A:266:VAL:HB	1:A:267:PRO:HD3	1.99	0.45
1:A:222:SER:O	1:A:225:SER:OG	2.28	0.44
1:A:446:THR:HG22	1:A:446:THR:O	2.17	0.44
1:A:234:PRO:HA	1:A:235:PRO:HD2	1.85	0.44
2:B:530:LEU:HD21	2:B:635:LEU:HD11	1.99	0.44
2:B:518:GLU:OE2	2:B:521:ARG:HD2	2.17	0.44
1:A:131:LYS:HD3	6:A:507:SO4:O2	2.17	0.44
1:A:261:HIS:CE1	1:A:344:LEU:HD12	2.53	0.44
1:A:218:ARG:NH2	2:B:606:GLN:OE1	2.26	0.43
2:B:554:LEU:HD22	2:B:599:VAL:HG21	2.00	0.43
2:B:581:LEU:O	2:B:582:ASN:C	2.62	0.43
1:A:29:HIS:HD2	1:A:424:VAL:HG13	1.83	0.43
1:A:360:SER:HA	9:A:602:HOH:O	2.19	0.42
2:B:502:MET:HE3	2:B:502:MET:HB2	1.80	0.42
2:B:664:LYS:HD3	2:B:674:VAL:CG1	2.50	0.41
1:A:29:HIS:CD2	1:A:424:VAL:HG13	2.54	0.41
1:A:243:THR:OG1	1:A:415:GLY:HA3	2.21	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	446/449 (99%)	430 (96%)	14 (3%)	2 (0%)	30	10
2	B	191/194 (98%)	185 (97%)	6 (3%)	0	100	100
All	All	637/643 (99%)	615 (96%)	20 (3%)	2 (0%)	36	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	A	235	PRO

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	367/369 (100%)	358 (98%)	9 (2%)	42	11
2	B	172/173 (99%)	162 (94%)	10 (6%)	18	1
All	All	539/542 (99%)	520 (96%)	19 (4%)	32	6

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	78	LEU
1	A	121	LYS
1	A	131	LYS
1	A	219	SER
1	A	236	GLU
1	A	240	LEU
1	A	298	CYS
1	A	366	MET
2	B	506	GLN
2	B	508	ASP
2	B	521	ARG
2	B	524	ASN
2	B	532	GLN

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Mol	Chain	Res	Type
2	B	554	LEU
2	B	571	LEU
2	B	581	LEU
2	B	593	GLN
2	B	690	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	115	GLN
2	B	506	GLN
2	B	514	HIS
2	B	526	HIS
2	B	556	HIS
2	B	582	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	501	-	3,3,3	0.35	0	2,2,2	0.38	0
4	IND	A	505	-	10,10,10	1.53	2 (20%)	13,13,13	3.48	9 (69%)
3	EDO	A	502	-	3,3,3	0.31	0	2,2,2	0.97	0
3	EDO	A	504	-	3,3,3	0.29	0	2,2,2	0.12	0
6	SO4	A	507	-	4,4,4	0.20	0	6,6,6	0.46	0
3	EDO	A	503	-	3,3,3	0.35	0	2,2,2	0.20	0
3	EDO	B	701	-	3,3,3	0.34	0	2,2,2	0.55	0
3	EDO	B	705	-	3,3,3	0.25	0	2,2,2	0.41	0
5	OXY	A	506	8	1,1,1	1.09	0	-		
6	SO4	B	703	-	4,4,4	0.22	0	6,6,6	0.45	0
3	EDO	A	510	-	3,3,3	0.26	0	2,2,2	0.58	0
7	FES	A	508	1	0,4,4	-	-	-		
6	SO4	B	702	-	4,4,4	0.27	0	6,6,6	0.06	0
6	SO4	B	704	-	4,4,4	0.42	0	6,6,6	0.38	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	501	-	-	0/1/1/1	-
4	IND	A	505	-	-	-	0/2/2/2
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	B	701	-	-	0/1/1/1	-
3	EDO	B	705	-	-	0/1/1/1	-
3	EDO	A	510	-	-	0/1/1/1	-
7	FES	A	508	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	IND	C9-C8	3.66	1.46	1.41
4	A	505	IND	C2-C3	2.06	1.40	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	IND	C8-C9-C3	7.73	111.48	106.59
4	A	505	IND	C9-C3-C2	-4.72	101.30	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	IND	C9-C8-N1	-4.44	103.97	107.53
4	A	505	IND	C7-C8-N1	3.85	136.90	130.74
4	A	505	IND	C7-C8-C9	-3.32	119.12	122.13
4	A	505	IND	C4-C9-C3	-2.83	126.94	134.97
4	A	505	IND	C3-C2-N1	2.30	112.90	110.25
4	A	505	IND	C5-C4-C9	-2.22	117.60	120.95
4	A	505	IND	C4-C9-C8	2.18	121.58	119.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	EDO	O1-C1-C2-O2
3	A	502	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
6	A	507	SO4	1	0
3	A	510	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, 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	448/449 (99%)	0.81	55 (12%) 8 9	11, 17, 30, 48	0
2	B	193/194 (99%)	0.87	29 (15%) 5 6	11, 16, 33, 45	0
All	All	641/643 (99%)	0.83	84 (13%) 7 8	11, 16, 31, 48	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	525	CYS	8.0
1	A	225	SER	6.7
1	A	447	THR	6.1
1	A	224	PHE	5.9
1	A	235	PRO	5.6
2	B	502	MET	5.3
1	A	236	GLU	4.8
1	A	3	TYR	4.5
1	A	298	CYS	4.4
1	A	220	GLY	4.3
1	A	446	THR	4.3
2	B	523	PHE	4.0
1	A	223	ILE	4.0
2	B	629	VAL	3.9
1	A	394	TYR	3.8
1	A	132	CYS	3.8
2	B	577	ARG	3.7
1	A	219	SER	3.7
1	A	282	LYS	3.7
2	B	524	ASN	3.4
1	A	226	SER	3.2
2	B	506	GLN	3.2
1	A	127	SER	3.1
2	B	520	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	527	ASP	3.0
1	A	234	PRO	3.0
2	B	530	LEU	3.0
1	A	121	LYS	3.0
2	B	526	HIS	2.9
2	B	532	GLN	2.9
2	B	580	LYS	2.9
2	B	503	ILE	2.8
1	A	237	GLY	2.8
1	A	285	GLY	2.8
2	B	519	ILE	2.8
1	A	398	VAL	2.7
1	A	264	ASP	2.7
2	B	575	SER	2.7
2	B	630	ASN	2.6
1	A	260	VAL	2.6
2	B	670	VAL	2.6
2	B	669	GLY	2.6
1	A	227	LEU	2.6
2	B	581	LEU	2.6
1	A	221	GLU	2.6
1	A	1	MET	2.5
1	A	287	VAL	2.5
1	A	125	GLY	2.5
1	A	262	SER	2.5
1	A	391	GLU	2.5
1	A	358	TRP	2.5
1	A	126	GLU	2.4
1	A	342	ARG	2.4
1	A	278	GLU	2.4
1	A	160	MET	2.4
1	A	222	SER	2.4
2	B	578	ARG	2.4
1	A	233	LEU	2.4
2	B	509	LYS	2.4
1	A	263	ALA	2.3
1	A	284	ILE	2.3
1	A	217	LEU	2.3
1	A	240	LEU	2.3
1	A	129	ASN	2.3
1	A	445	LYS	2.3
1	A	218	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	131	LYS	2.3
1	A	179	GLY	2.3
2	B	593	GLN	2.3
1	A	254	TRP	2.3
1	A	228	ALA	2.2
2	B	554	LEU	2.1
2	B	521	ARG	2.1
2	B	667	GLU	2.1
2	B	528	SER	2.1
1	A	122	ASP	2.1
1	A	231	ALA	2.1
1	A	280	LEU	2.1
2	B	507	GLU	2.1
1	A	210	GLY	2.1
1	A	182	LEU	2.0
2	B	551	ARG	2.0
1	A	47	LEU	2.0
1	A	123	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(Å ²)	Q<0.9
6	SO4	B	702	5/5	0.74	0.21	76,76,76,77	0
5	OXY	A	506	2/2	0.77	0.20	32,32,32,39	0
3	EDO	A	503	4/4	0.77	0.26	24,33,35,40	0
3	EDO	A	504	4/4	0.79	0.19	33,33,33,34	0
4	IND	A	505	9/9	0.83	0.13	31,32,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	A	507	5/5	0.87	0.14	40,43,44,44	0
3	EDO	A	502	4/4	0.92	0.10	14,21,21,23	0
3	EDO	B	705	4/4	0.92	0.11	14,23,27,31	0
3	EDO	A	510	4/4	0.94	0.10	26,26,28,29	0
6	SO4	B	704	5/5	0.94	0.13	27,33,36,37	5
6	SO4	B	703	5/5	0.95	0.11	24,26,33,33	0
3	EDO	B	701	4/4	0.95	0.08	16,16,17,18	0
3	EDO	A	501	4/4	0.98	0.04	13,13,15,16	0
7	FES	A	508	4/4	0.99	0.03	13,13,14,15	0
8	FE	A	509	1/1	0.99	0.16	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.