Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 08:04 PM UTC

PDB ID	:	4HM0 / pdb_00004hm0
Title	:	Naphthalene 1,2-Dioxygenase bound to indole-3-acetate
Authors	:	Ferraro, D.J.; Ramaswamy, S.
Deposited on	:	2012-10-17
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

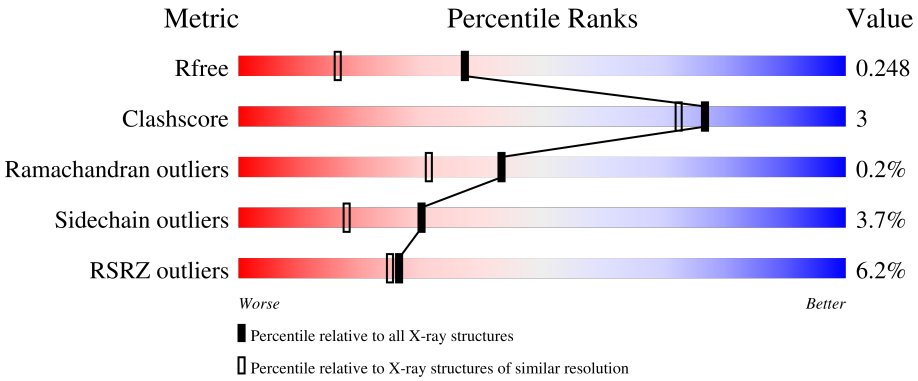
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 <=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	6% 91% 8% ·
2	B	194	6% 88% 10% •••

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5655 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.

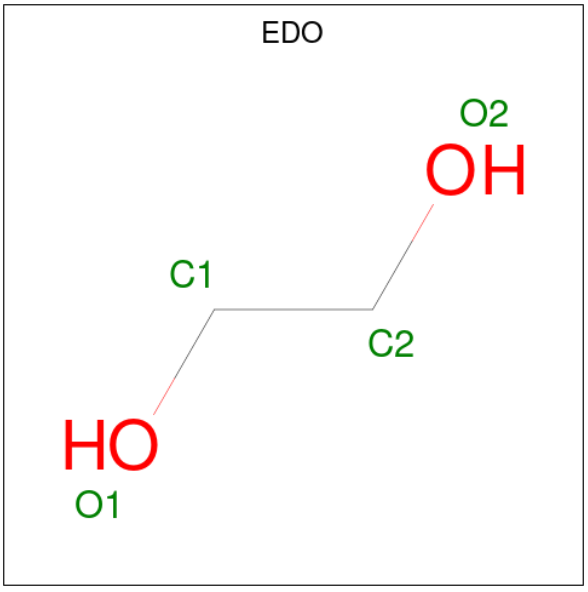
- Molecule 1 is a protein called Naphthalene 1,2-dioxygenase subunit alpha.

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 subunit beta.

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: $C_2H_6O_2$).



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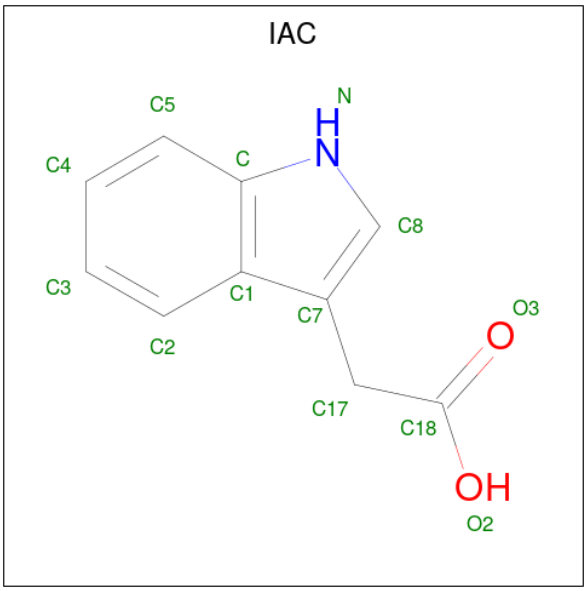
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

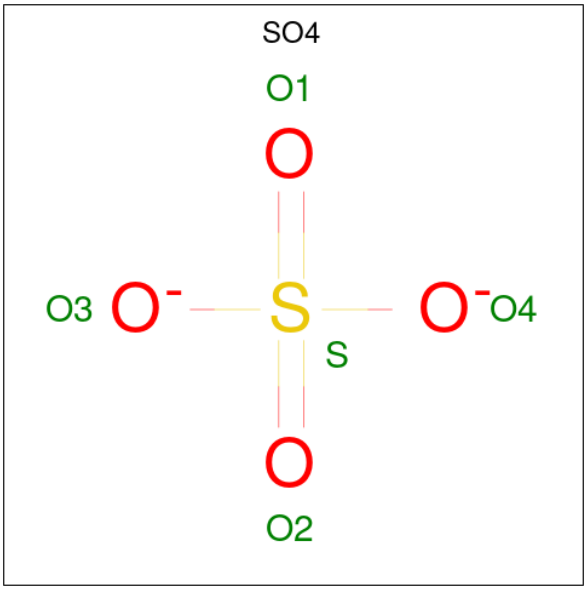
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is 1H-INDOL-3-YLACETIC ACID (CCD ID: IAC) (formula: $C_{10}H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			13	10	1	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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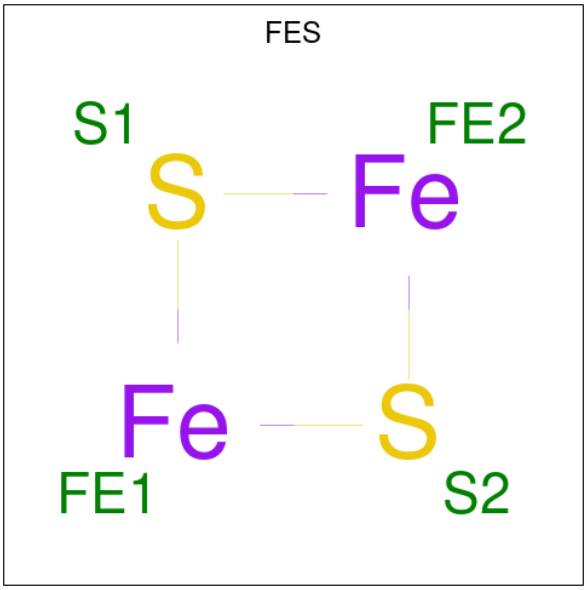
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- 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 4 2 2	0	0

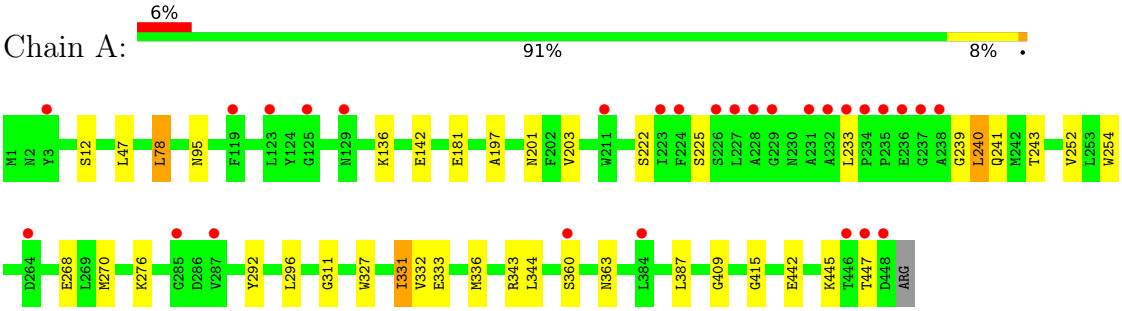
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	312	Total O 312 312	0	0
8	B	151	Total O 151 151	0	0

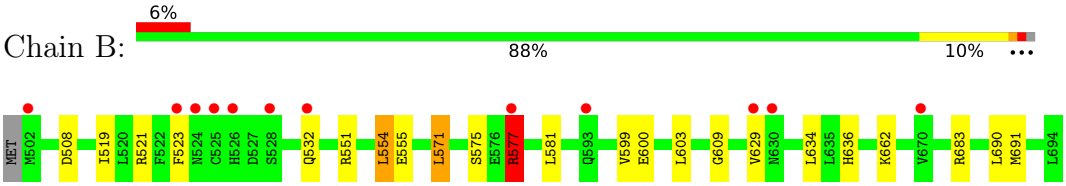
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Naphthalene 1,2-dioxygenase subunit alpha



• Molecule 2: Naphthalene 1,2-dioxygenase subunit beta



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	140.68Å 140.68Å 207.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.61 – 1.80 40.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.8 (40.61-1.80) 85.3 (40.61-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.214 , 0.254 0.207 , 0.248	Depositor DCC
R_{free} test set	3157 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5655	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.48	0/3573	0.81	3/4841 (0.1%)
2	B	0.48	0/1638	0.77	0/2209
All	All	0.48	0/5211	0.79	3/7050 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	445	LYS	N-CA-C	8.78	121.95	111.33
1	A	197	ALA	CA-C-N	-6.22	113.28	119.56
1	A	197	ALA	C-N-CA	-6.22	113.28	119.56

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	20	0
2	B	1608	0	1583	11	0
3	A	36	0	54	3	1
3	B	24	0	36	0	0
4	A	1	0	0	0	0
5	A	13	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	15	0	0	0	0
6	B	10	0	0	0	0
7	A	4	0	0	0	0
8	A	312	0	0	2	1
8	B	151	0	0	2	0
All	All	5655	0	4997	29	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 (29) 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:270:MET:SD	8:A:617:HOH:O	2.53	0.65
1:A:387:LEU:HG	1:A:409:GLY:HA2	1.84	0.60
1:A:78:LEU:HD22	1:A:136:LYS:HD3	1.84	0.58
1:A:270:MET:HG3	8:A:609:HOH:O	2.08	0.54
2:B:551:ARG:NH1	2:B:600:GLU:OE1	2.33	0.53
2:B:554:LEU:HD22	2:B:599:VAL:HG21	1.93	0.51
1:A:268:GLU:CD	1:A:343:ARG:HH22	2.18	0.51
2:B:571:LEU:HD22	2:B:683:ARG:HG2	1.93	0.50
1:A:311:GLY:HA2	1:A:331:ILE:HG13	1.92	0.50
1:A:332:VAL:HG12	1:A:344:LEU:HD23	1.94	0.50
1:A:142:GLU:HG2	3:A:512:EDO:H21	1.94	0.50
1:A:222:SER:O	1:A:225:SER:OG	2.19	0.50
1:A:95:ASN:O	2:B:577:ARG:NH2	2.45	0.49
2:B:634:LEU:HD11	2:B:662:LYS:HG2	1.96	0.48
3:A:511:EDO:H21	2:B:609:GLY:N	2.29	0.47
1:A:240:LEU:HD13	1:A:252:VAL:HB	1.96	0.46
1:A:276:LYS:HD2	1:A:292:TYR:CZ	2.51	0.46
2:B:575:SER:O	2:B:577:ARG:HD3	2.15	0.46
1:A:201:ASN:ND2	5:A:505:IAC:O3	2.47	0.46
1:A:327:TRP:CZ3	3:A:510:EDO:H12	2.52	0.45
1:A:252:VAL:HG22	1:A:296:LEU:HD22	1.99	0.43
1:A:243:THR:OG1	1:A:415:GLY:HA3	2.19	0.42
1:A:239:GLY:HA2	1:A:254:TRP:CD1	2.54	0.42
2:B:523:PHE:HE1	8:B:812:HOH:O	2.04	0.41
1:A:360:SER:OG	2:B:691:MET:HE2	2.20	0.41
2:B:521:ARG:HD3	2:B:636:HIS:CG	2.56	0.41
2:B:555:GLU:HG3	8:B:926:HOH:O	2.20	0.41
1:A:333:GLU:HB2	1:A:336:MET:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:SER:HA	1:A:442:GLU:HG2	2.04	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)
3:A:511:EDO:O2	8:A:603:HOH:O[3_565]	2.04	0.16

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%)	436 (98%)	10 (2%)	0	100	100
2	B	191/194 (98%)	187 (98%)	3 (2%)	1 (0%)	24	14
All	All	637/643 (99%)	623 (98%)	13 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	577	ARG

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	367/369 (100%)	357 (97%)	10 (3%)	39 27
2	B	172/173 (99%)	162 (94%)	10 (6%)	18 7
All	All	539/542 (99%)	519 (96%)	20 (4%)	30 18

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	78	LEU
1	A	181	GLU
1	A	203	VAL
1	A	233	LEU
1	A	240	LEU
1	A	241	GLN
1	A	331	ILE
1	A	363	ASN
1	A	447	THR
2	B	508	ASP
2	B	519	ILE
2	B	532	GLN
2	B	554	LEU
2	B	571	LEU
2	B	577	ARG
2	B	581	LEU
2	B	603	LEU
2	B	629	VAL
2	B	690	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	A	28	GLN
2	B	514	HIS
2	B	593	GLN

5.3.3 RNA

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 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	B	704	-	3,3,3	0.56	0	2,2,2	0.13	0
3	EDO	A	511	-	3,3,3	0.24	0	2,2,2	0.33	0
6	SO4	B	708	-	4,4,4	0.25	0	6,6,6	0.15	0
3	EDO	A	514	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	B	706	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	A	512	-	3,3,3	0.36	0	2,2,2	0.65	0
3	EDO	B	705	-	3,3,3	0.45	0	2,2,2	0.43	0
6	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.26	0
6	SO4	A	507	-	4,4,4	0.24	0	6,6,6	0.06	0
3	EDO	B	707	-	3,3,3	0.32	0	2,2,2	0.58	0
3	EDO	A	501	-	3,3,3	0.45	0	2,2,2	0.14	0
6	SO4	B	702	-	4,4,4	0.20	0	6,6,6	0.14	0
3	EDO	A	513	-	3,3,3	0.42	0	2,2,2	0.46	0
7	FES	A	508	1	0,4,4	-	-	-		
6	SO4	A	515	-	4,4,4	0.28	0	6,6,6	0.21	0
5	IAC	A	505	4	14,14,14	1.07	0	19,19,19	2.44	5 (26%)
3	EDO	A	509	-	3,3,3	0.44	0	2,2,2	0.56	0
3	EDO	A	510	-	3,3,3	0.44	0	2,2,2	0.39	0
3	EDO	A	503	-	3,3,3	0.47	0	2,2,2	0.33	0
3	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.16	0
3	EDO	B	703	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	B	701	-	3,3,3	0.50	0	2,2,2	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
7	FES	A	508	1	-	-	0/1/1/1
3	EDO	A	514	-	-	0/1/1/1	-
3	EDO	B	706	-	-	0/1/1/1	-
3	EDO	B	704	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	A	501	-	-	0/1/1/1	-
3	EDO	B	703	-	-	0/1/1/1	-
3	EDO	B	707	-	-	1/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	A	511	-	-	0/1/1/1	-
5	IAC	A	505	4	-	0/4/4/4	0/2/2/2
3	EDO	B	701	-	-	0/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
3	EDO	B	705	-	-	1/1/1/1	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	505	IAC	C18-C17-C7	-6.19	105.44	114.93
5	A	505	IAC	C2-C1-C	4.87	123.89	118.84
5	A	505	IAC	C5-C-C1	-3.88	118.44	122.19
5	A	505	IAC	C2-C1-C7	-2.64	129.91	133.85
5	A	505	IAC	C-N-C8	2.52	111.32	109.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	513	EDO	O1-C1-C2-O2
3	A	510	EDO	O1-C1-C2-O2
3	A	509	EDO	O1-C1-C2-O2
3	A	512	EDO	O1-C1-C2-O2
3	B	704	EDO	O1-C1-C2-O2
3	B	705	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	707	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	511	EDO	1	1
3	A	512	EDO	1	0
5	A	505	IAC	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	448/449 (99%)	0.51	28 (6%)	26	24	20, 27, 45, 65	0
2	B	193/194 (99%)	0.31	12 (6%)	26	25	17, 24, 47, 58	0
All	All	641/643 (99%)	0.45	40 (6%)	26	25	17, 27, 45, 65	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	PRO	5.6
2	B	523	PHE	5.2
1	A	233	LEU	4.8
1	A	446	THR	4.5
2	B	577	ARG	4.4
1	A	447	THR	4.3
1	A	119	PHE	4.2
1	A	234	PRO	4.2
1	A	232	ALA	3.9
2	B	528	SER	3.7
2	B	524	ASN	3.6
1	A	125	GLY	3.6
1	A	223	ILE	3.4
1	A	129	ASN	3.4
2	B	629	VAL	3.3
1	A	236	GLU	3.2
1	A	226	SER	3.2
1	A	237	GLY	3.2
2	B	502	MET	3.0
2	B	526	HIS	3.0
2	B	525	CYS	3.0
2	B	532	GLN	3.0
1	A	448	ASP	3.0
1	A	228	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	231	ALA	2.8
1	A	227	LEU	2.8
1	A	224	PHE	2.6
1	A	384	LEU	2.6
1	A	123	LEU	2.5
1	A	360	SER	2.5
1	A	238	ALA	2.4
1	A	285	GLY	2.4
2	B	593	GLN	2.4
1	A	287	VAL	2.2
2	B	630	ASN	2.2
1	A	3	TYR	2.2
1	A	264	ASP	2.2
1	A	229	GLY	2.1
1	A	211	TRP	2.1
2	B	670	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	B	708	5/5	0.66	0.15	48,51,55,60	0
3	EDO	A	513	4/4	0.78	0.15	31,35,40,41	0
3	EDO	B	704	4/4	0.79	0.20	38,42,42,43	0
3	EDO	A	512	4/4	0.79	0.15	35,39,43,44	0
6	SO4	A	515	5/5	0.80	0.12	45,47,53,55	0
6	SO4	A	506	5/5	0.80	0.13	37,44,51,55	0
6	SO4	A	507	5/5	0.82	0.13	47,49,57,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	701	4/4	0.84	0.18	31,32,34,39	0
3	EDO	A	503	4/4	0.84	0.13	33,39,40,41	0
3	EDO	A	514	4/4	0.88	0.13	33,37,37,39	0
3	EDO	B	707	4/4	0.88	0.17	22,29,31,35	0
3	EDO	A	509	4/4	0.89	0.12	26,32,36,37	0
3	EDO	A	510	4/4	0.89	0.13	25,29,30,31	0
3	EDO	A	502	4/4	0.91	0.10	27,30,33,33	0
5	IAC	A	505	13/13	0.91	0.10	30,32,36,37	0
3	EDO	B	706	4/4	0.91	0.11	23,27,29,40	0
3	EDO	A	511	4/4	0.92	0.14	24,33,36,38	0
6	SO4	B	702	5/5	0.93	0.07	41,43,48,49	0
3	EDO	B	705	4/4	0.93	0.12	22,26,29,39	0
3	EDO	B	703	4/4	0.95	0.07	21,23,23,24	0
3	EDO	A	501	4/4	0.97	0.06	20,24,25,25	0
4	FE	A	504	1/1	0.99	0.03	31,31,31,31	0
7	FES	A	508	4/4	0.99	0.03	22,24,24,26	0

6.5 Other polymers (i)

There are no such residues in this entry.