Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 03:05 am BST

PDB ID	:	2BMR / pdb_00002bmr
Title	:	The Crystal Structure of Nitrobenzene Dioxygenase in complex with 3- nitrotoluene
Authors	:	Friemann, R.; Ivkovic-Jensen, M.M.; Lessner, D.J.; Yu, C.; Gibson, D.T.; Parales, R.E.; Eklund, H.; Ramaswamy, S.
Deposited on	:	2005-03-15
Resolution	:	1.50 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:

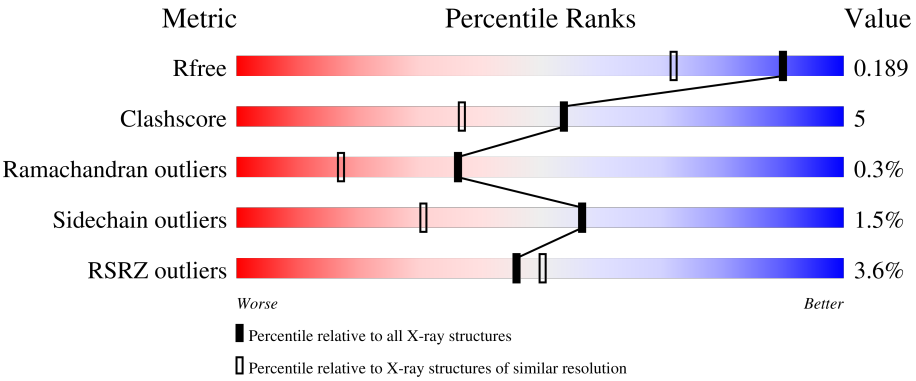
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	447	3% 90% 8%
2	B	194	5% 88% 10%

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
7	EOH	A	1446	-	-	X	-
7	EOH	A	1447	-	-	X	-
7	EOH	B	1201	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6127 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.

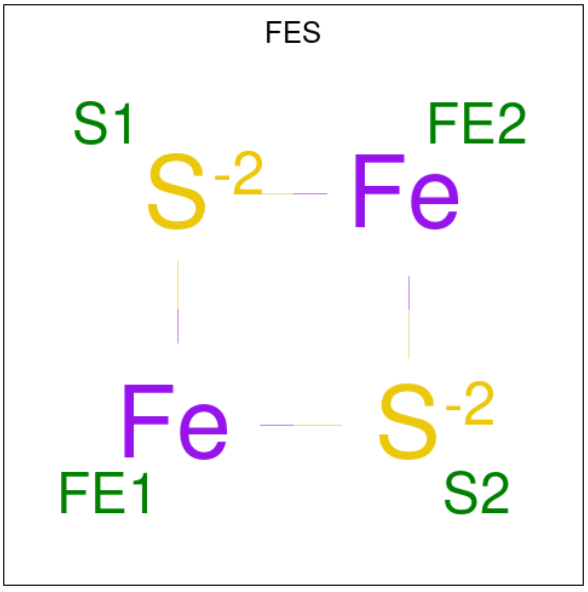
- Molecule 1 is a protein called OXYGENASE-ALPHA NBDO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3577	2281	611	671	14	46	21	0

- Molecule 2 is a protein called OXYGENASE-BETA NBDO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	194	1755	1104	324	322	5	20	15	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

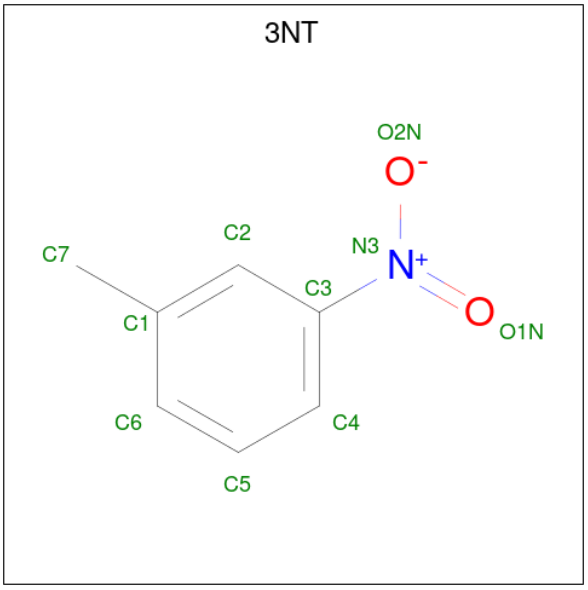


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0

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

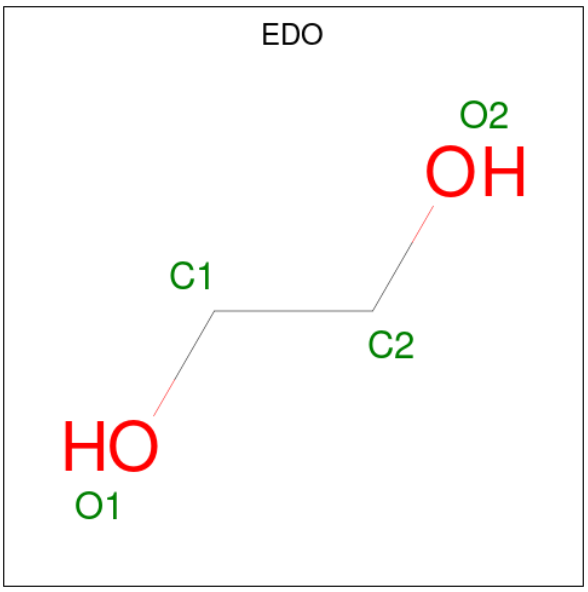
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0

- Molecule 5 is 3-NITROTOLUENE (CCD ID: 3NT) (formula: $C_7H_7NO_2$).



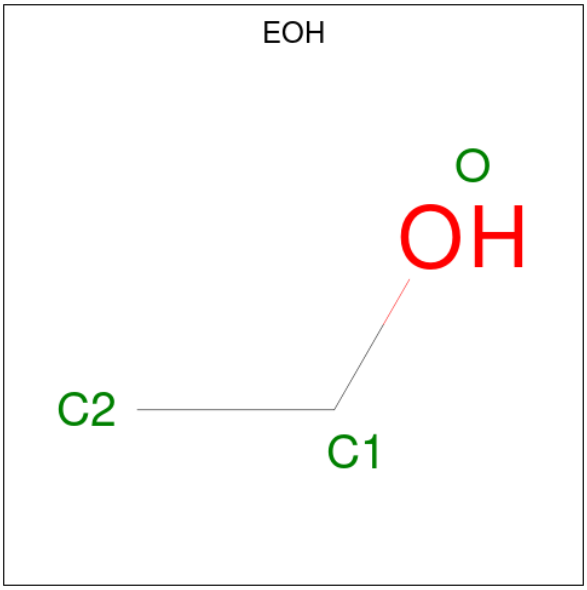
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 10 7 1 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



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

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

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total Ni 2 2	0	0

- Molecule 9 is water.

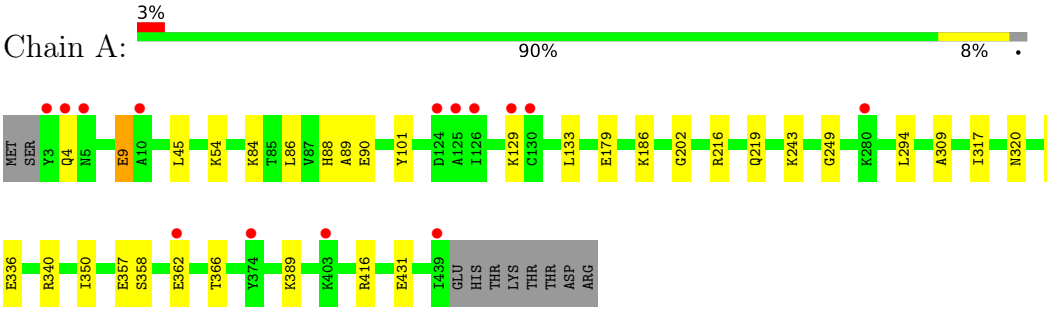
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	425	Total O 425 425	0	0
9	B	302	Total O 302 302	0	0

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.

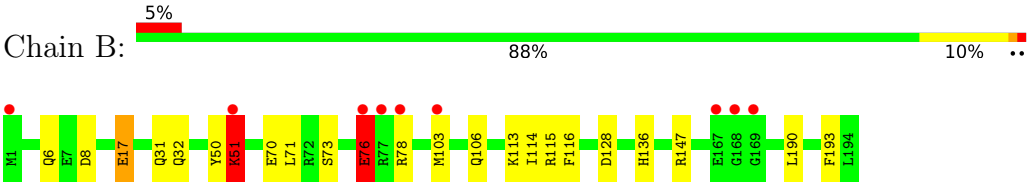
• Molecule 1: OXYGENASE-ALPHA NBDO

Chain A:



• Molecule 2: OXYGENASE-BETA NBDO

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	121.62Å 121.62Å 84.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.55 – 1.50 52.55 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (52.55-1.50) 98.4 (52.55-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.169 , 0.191 0.168 , 0.189	Depositor DCC
R_{free} test set	5562 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6127	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: 3NT, EDO, EOH, FE, FES, NI

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	0.55	0/3672	0.76	1/4964 (0.0%)
2	B	3.55	4/1791 (0.2%)	1.15	14/2417 (0.6%)
All	All	2.08	4/5463 (0.1%)	0.90	15/7381 (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
2	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	51[A]	LYS	CE-NZ	77.38	3.81	1.49
2	B	51[B]	LYS	CE-NZ	77.38	3.81	1.49
2	B	51[A]	LYS	CD-CE	71.20	3.66	1.52
2	B	51[B]	LYS	CD-CE	71.20	3.66	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	51[A]	LYS	CD-CE-NZ	-22.68	39.31	111.90
2	B	51[B]	LYS	CD-CE-NZ	-22.68	39.31	111.90
2	B	51[A]	LYS	CG-CD-CE	-11.56	84.72	111.30
2	B	51[B]	LYS	CG-CD-CE	-11.56	84.72	111.30
2	B	6	GLN	OE1-CD-NE2	-10.14	112.46	122.60
2	B	32[A]	GLN	OE1-CD-NE2	-9.53	113.07	122.60
2	B	32[B]	GLN	OE1-CD-NE2	-9.53	113.07	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	76[A]	GLU	CA-C-N	6.97	134.35	121.52
2	B	76[A]	GLU	C-N-CA	6.97	134.35	121.52
2	B	76[B]	GLU	CA-C-N	6.97	134.35	121.52
2	B	76[B]	GLU	C-N-CA	6.97	134.35	121.52
2	B	6	GLN	CG-CD-NE2	6.88	126.72	116.40
1	A	9	GLU	N-CA-CB	6.49	119.58	110.04
2	B	32[A]	GLN	CG-CD-NE2	6.31	125.86	116.40
2	B	32[B]	GLN	CG-CD-NE2	6.31	125.86	116.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	51[B]	LYS	Mainchain
2	B	76[B]	GLU	Mainchain

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	3577	0	3423	30	0
2	B	1755	0	1719	21	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
5	A	10	0	7	0	0
6	A	12	0	18	2	0
6	B	12	0	16	1	0
7	A	15	0	30	14	0
7	B	12	0	24	4	0
8	B	2	0	0	0	0
9	A	425	0	0	7	0
9	B	302	0	0	4	0
All	All	6127	0	5237	52	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 5.

All (52) 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)
2:B:50:TYR:C	2:B:51[B]:LYS:N	1.74	1.42
1:A:186:LYS:HZ1	7:A:1447:EOH:H22	1.44	0.82
7:A:1448:EOH:H22	9:A:2179:HOH:O	1.80	0.80
2:B:50:TYR:C	2:B:51[B]:LYS:CA	2.41	0.78
1:A:54[B]:LYS:HD3	1:A:89:ALA:O	1.86	0.75
1:A:336[B]:GLU:HG3	1:A:340:ARG:NH1	2.04	0.71
1:A:320:ASN:CG	9:A:2319:HOH:O	2.32	0.71
1:A:90:GLU:HG2	7:A:1447:EOH:H21	1.71	0.71
1:A:54[A]:LYS:HB3	7:A:1447:EOH:H23	1.74	0.70
1:A:179:GLU:HG3	1:A:332:LYS:HG2	1.74	0.69
2:B:128:ASP:OD1	2:B:136:HIS:HE1	1.77	0.68
1:A:186:LYS:NZ	7:A:1447:EOH:H22	2.09	0.67
1:A:54[A]:LYS:NZ	7:A:1447:EOH:H12	2.10	0.67
1:A:54[A]:LYS:HZ2	7:A:1447:EOH:H12	1.60	0.67
1:A:243:LYS:O	1:A:416[B]:ARG:NH2	2.25	0.66
7:A:1446:EOH:H21	9:B:2160:HOH:O	1.97	0.65
1:A:362:GLU:O	1:A:366[B]:THR:HB	1.97	0.64
1:A:86[B]:LEU:HD11	1:A:133:LEU:HD21	1.82	0.61
2:B:50:TYR:C	2:B:51[B]:LYS:C	2.68	0.61
2:B:115:ARG:HE	7:B:1201:EOH:H21	1.66	0.60
2:B:113:LYS:O	7:B:1200:EOH:H11	2.01	0.60
1:A:54[B]:LYS:O	7:A:1447:EOH:H23	2.03	0.59
1:A:431:GLU:OE1	7:A:1450:EOH:H21	2.04	0.57
2:B:73:SER:HB3	2:B:76[A]:GLU:HB2	1.86	0.56
1:A:320:ASN:ND2	9:A:2319:HOH:O	2.40	0.54
1:A:389:LYS:HD2	9:A:2163:HOH:O	2.08	0.53
2:B:51[B]:LYS:HG2	9:B:2126:HOH:O	2.09	0.53
2:B:50:TYR:CA	2:B:51[B]:LYS:N	2.68	0.52
7:A:1446:EOH:H22	2:B:70:GLU:OE2	2.10	0.52
2:B:50:TYR:O	2:B:51[B]:LYS:C	2.53	0.51
2:B:115:ARG:HE	7:B:1201:EOH:C2	2.23	0.51
1:A:216:ARG:NH2	2:B:106:GLN:OE1	2.41	0.49
6:A:1445:EDO:H22	7:A:1446:EOH:O	2.13	0.49
1:A:350:ILE:HA	1:A:357:GLU:HB2	1.94	0.49
2:B:136:HIS:HD2	9:B:2261:HOH:O	1.97	0.47
1:A:129:LYS:HG3	9:A:2154:HOH:O	2.13	0.47
2:B:17[A]:GLU:HG3	9:B:2034:HOH:O	2.14	0.47
1:A:90:GLU:HB3	6:A:1445:EDO:H11	1.96	0.46
1:A:45:LEU:HD13	7:A:1446:EOH:H12	1.97	0.45
1:A:86[B]:LEU:HD11	1:A:133:LEU:CD2	2.45	0.45
2:B:116:PHE:O	7:B:1201:EOH:H23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317[B]:ILE:HD11	1:A:323:GLU:HB2	1.99	0.44
1:A:216:ARG:NH2	2:B:106:GLN:HB2	2.34	0.43
1:A:219:GLN:NE2	9:A:2238:HOH:O	2.50	0.43
1:A:358[B]:SER:HB3	9:A:2346:HOH:O	2.19	0.43
1:A:249:GLY:O	1:A:294:LEU:HA	2.19	0.42
2:B:114[A]:ILE:HG23	2:B:147:ARG:HB3	2.00	0.42
1:A:84:LYS:HD2	1:A:101:TYR:HB2	2.02	0.41
2:B:193:PHE:CZ	6:B:1197:EDO:H11	2.55	0.41
1:A:88:HIS:HB2	7:A:1449:EOH:H23	2.02	0.41
2:B:73:SER:HB3	2:B:76[B]:GLU:HB2	2.04	0.40

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	456/447 (102%)	441 (97%)	13 (3%)	2 (0%)	30 12
2	B	207/194 (107%)	200 (97%)	7 (3%)	0	100 100
All	All	663/641 (103%)	641 (97%)	20 (3%)	2 (0%)	36 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	ALA
1	A	202	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	371/360 (103%)	369 (100%)	2 (0%)	81 66
2	B	191/177 (108%)	183 (96%)	8 (4%)	26 4
All	All	562/537 (105%)	552 (98%)	10 (2%)	57 24

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	9	GLU
2	B	8	ASP
2	B	17[A]	GLU
2	B	17[B]	GLU
2	B	71	LEU
2	B	78	ARG
2	B	103[A]	MET
2	B	103[B]	MET
2	B	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	113	GLN
1	A	199	ASN
1	A	219	GLN
1	A	320	ASN
1	A	438	HIS
2	B	26	HIS
2	B	31	GLN
2	B	48	GLN
2	B	102	GLN
2	B	110	ASN
2	B	122	ASN
2	B	136	HIS

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 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
7	EOH	B	1203	-	2,2,2	0.44	0	1,1,1	0.10	0
7	EOH	B	1202	-	2,2,2	0.46	0	1,1,1	0.03	0
6	EDO	B	1197	-	3,3,3	0.45	0	2,2,2	0.13	0
7	EOH	A	1447	-	2,2,2	0.43	0	1,1,1	0.13	0
7	EOH	A	1449	-	2,2,2	0.45	0	1,1,1	0.13	0
6	EDO	A	1445	-	3,3,3	0.45	0	2,2,2	0.25	0
6	EDO	A	1443	-	3,3,3	0.46	0	2,2,2	0.38	0
6	EDO	A	1444	-	3,3,3	0.47	0	2,2,2	0.39	0
7	EOH	A	1450	-	2,2,2	0.44	0	1,1,1	0.34	0
3	FES	A	1440	1	0,4,4	-	-	-		
6	EDO	B	1198	8	3,3,3	0.77	0	2,2,2	0.64	0
5	3NT	A	1442	-	9,10,10	1.38	1 (11%)	11,13,13	1.25	1 (9%)
7	EOH	B	1200	-	2,2,2	0.49	0	1,1,1	0.34	0
7	EOH	B	1201	-	2,2,2	0.47	0	1,1,1	0.25	0
7	EOH	A	1448	-	2,2,2	0.40	0	1,1,1	0.01	0
6	EDO	B	1199	-	3,3,3	0.50	0	2,2,2	0.34	0
7	EOH	A	1446	-	2,2,2	0.40	0	1,1,1	0.15	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
6	EDO	B	1197	-	-	0/1/1/1	-
6	EDO	A	1445	-	-	1/1/1/1	-
6	EDO	A	1443	-	-	0/1/1/1	-
6	EDO	A	1444	-	-	0/1/1/1	-
3	FES	A	1440	1	-	-	0/1/1/1
6	EDO	B	1198	8	-	1/1/1/1	-
5	3NT	A	1442	-	-	0/2/4/4	0/1/1/1
6	EDO	B	1199	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1442	3NT	C3-N3	-3.60	1.36	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1442	3NT	C4-C3-N3	3.62	122.10	119.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1445	EDO	O1-C1-C2-O2
6	B	1198	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1197	EDO	1	0
7	A	1447	EOH	7	0
7	A	1449	EOH	1	0
6	A	1445	EDO	2	0
7	A	1450	EOH	1	0
7	B	1200	EOH	1	0
7	B	1201	EOH	3	0
7	A	1448	EOH	1	0
7	A	1446	EOH	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	50:TYR	C	51[B]:LYS	N	1.74
1	B	51[B]:LYS	C	52:ALA	N	1.61

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	437/447 (97%)	0.16	14 (3%) 50 54	6, 14, 23, 38	39 (8%)
2	B	194/194 (100%)	-0.08	9 (4%) 37 41	4, 11, 19, 29	18 (9%)
All	All	631/641 (98%)	0.09	23 (3%) 46 50	4, 13, 22, 38	57 (9%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51[A]	LYS	5.0
1	A	124	ASP	4.8
2	B	77	ARG	3.9
1	A	129	LYS	3.6
1	A	3	TYR	3.6
1	A	439	ILE	3.4
2	B	169	GLY	3.4
2	B	168	GLY	3.3
2	B	103[A]	MET	3.2
2	B	76[A]	GLU	3.2
1	A	125	ALA	3.1
1	A	4	GLN	3.0
1	A	10	ALA	2.9
1	A	280	LYS	2.9
2	B	78	ARG	2.8
2	B	1	MET	2.6
2	B	167	GLU	2.6
1	A	130	CYS	2.4
1	A	5	ASN	2.4
1	A	126	ILE	2.3
1	A	362	GLU	2.2
1	A	403[A]	LYS	2.1
1	A	374	TYR	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 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	EDO	B	1199	4/4	0.68	0.21	42,42,42,43	0
5	3NT	A	1442	10/10	0.76	0.17	28,29,32,34	0
7	EOH	B	1201	3/3	0.76	0.18	24,24,26,26	0
7	EOH	A	1450	3/3	0.78	0.20	32,32,33,33	0
6	EDO	A	1445	4/4	0.80	0.17	25,29,29,30	0
7	EOH	A	1446	3/3	0.81	0.19	14,14,19,21	0
7	EOH	B	1203	3/3	0.81	0.16	29,29,29,29	0
7	EOH	B	1200	3/3	0.82	0.17	18,18,20,21	0
7	EOH	B	1202	3/3	0.84	0.19	31,31,31,31	0
7	EOH	A	1447	3/3	0.88	0.19	21,21,21,23	0
6	EDO	B	1198	4/4	0.88	0.16	15,19,22,23	0
7	EOH	A	1449	3/3	0.90	0.14	24,24,24,25	0
4	FE	A	1441	1/1	0.92	0.07	18,18,18,18	0
6	EDO	B	1197	4/4	0.92	0.17	19,19,19,19	0
6	EDO	A	1444	4/4	0.92	0.11	25,28,28,29	0
7	EOH	A	1448	3/3	0.93	0.11	16,16,19,19	0
6	EDO	A	1443	4/4	0.95	0.12	20,23,23,23	0
8	NI	B	1195	1/1	0.99	0.02	14,14,14,14	1
8	NI	B	1196	1/1	0.99	0.06	9,9,9,9	1
3	FES	A	1440	4/4	1.00	0.02	12,12,12,13	0

6.5 Other polymers (i)

There are no such residues in this entry.