Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 05:47 am BST

PDB ID	:	1UUV / pdb_00001uuv
Title	:	NAPHTHALENE 1,2-DIOXYGENASE WITH NITRIC OXIDE AND INDOLE BOUND IN THE ACTIVE SITE.
Authors	:	Karlsson, A.; Parales, J.V.; Parales, R.E.; Gibson, D.T.; Eklund, H.; Ramaswamy, S.
Deposited on	:	2004-01-11
Resolution	:	1.65 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:

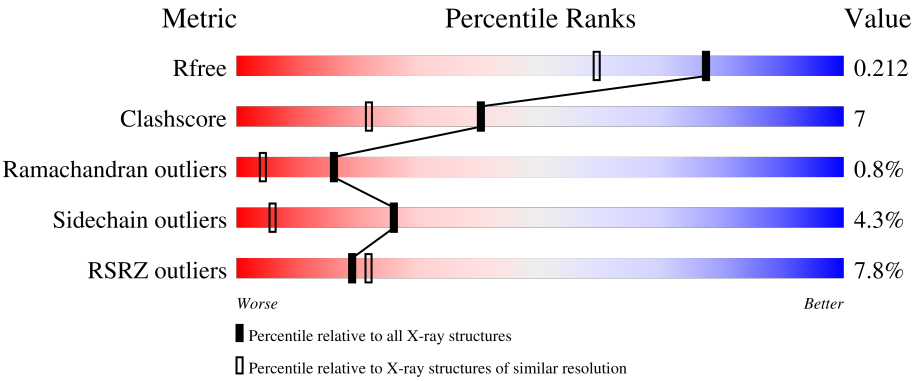
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.65 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 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	9% 89% 9%
2	B	194	6% 82% 14%

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	EDO	A	1451	-	-	X	-
8	SO4	B	1699	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5601 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.

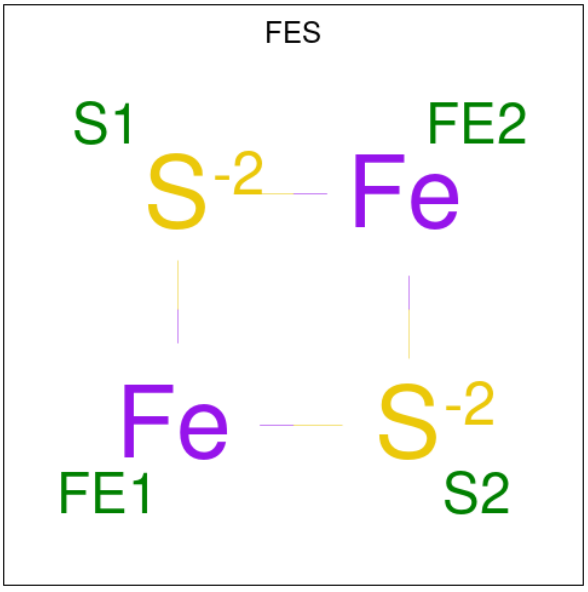
- Molecule 1 is a protein called NAPHTHALENE 1,2-DIOXYGENASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	447	3480	2202	597	665	16	0	0	0

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

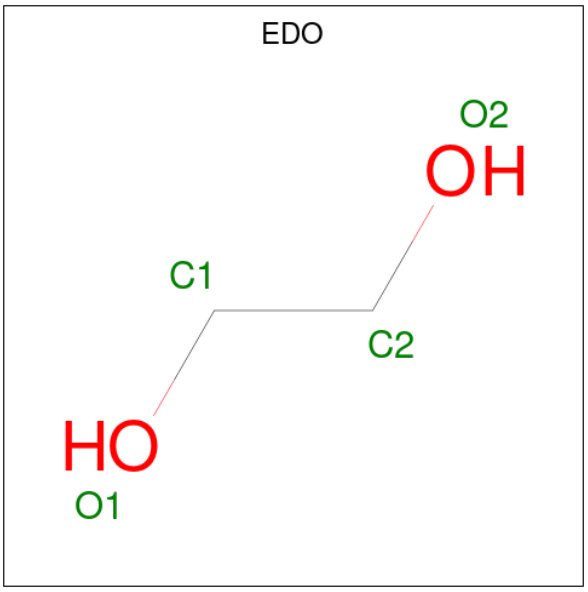
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	193	1607	1007	302	292	6	0	0	0

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



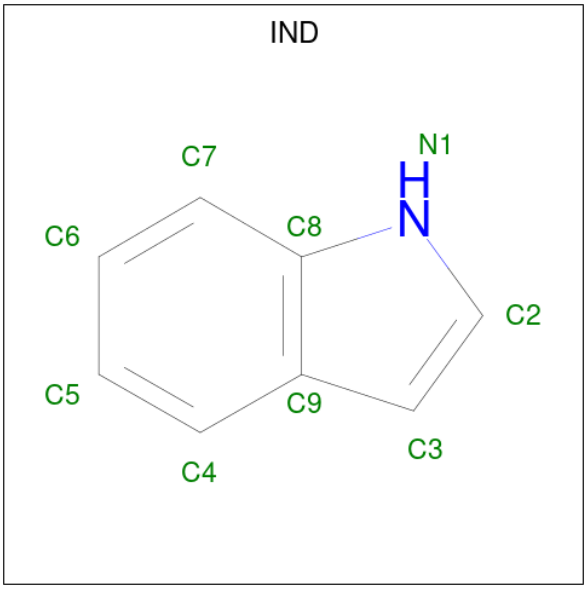
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	4	2	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



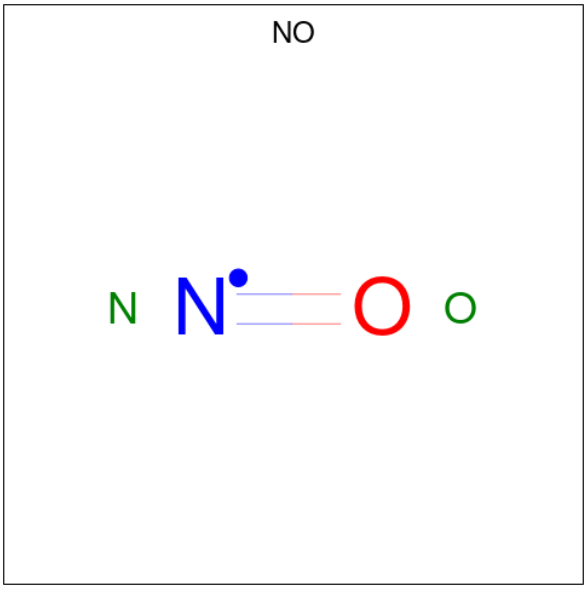
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is INDOLE (CCD ID: IND) (formula: C_8H_7N).



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

- Molecule 6 is NITRIC OXIDE (CCD ID: NO) (formula: NO).

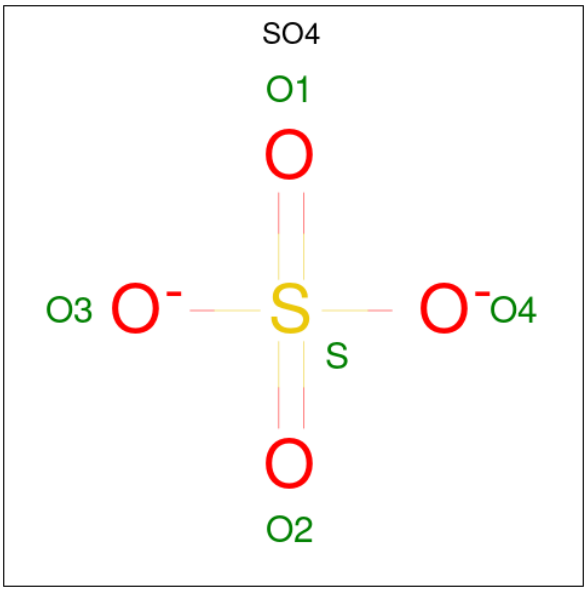


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total N O 2 1 1	0	0

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

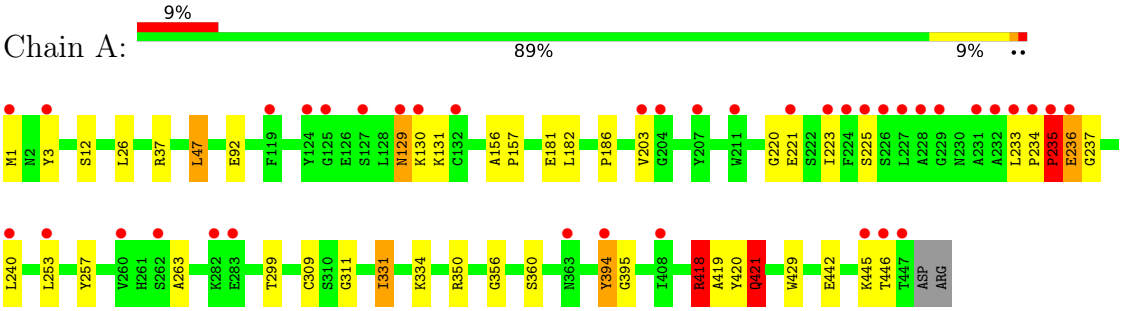
- Molecule 9 is water.

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

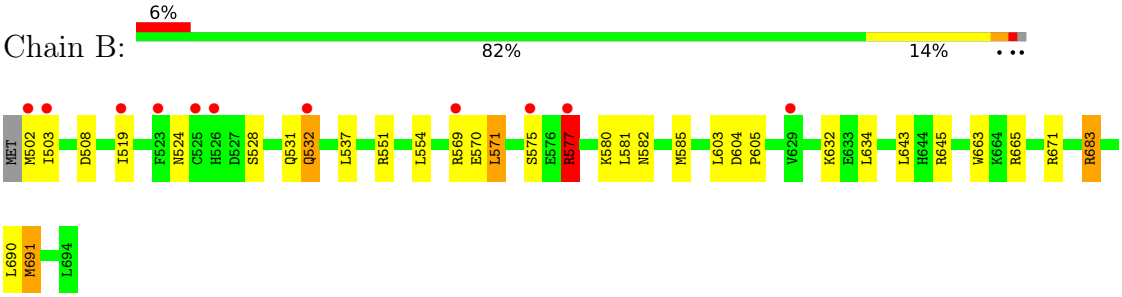
3 Residue-property plots (i)

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 ALPHA SUBUNIT



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	139.60Å 139.60Å 209.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.65 25.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (25.00-1.65) 98.3 (25.00-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.0.36	Depositor
R, R_{free}	0.184 , 0.204 0.192 , 0.212	Depositor DCC
R_{free} test set	4634 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5601	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: SO4, EDO, NO, 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	0.82	4/3572 (0.1%)	1.06	12/4839 (0.2%)
2	B	0.76	1/1637 (0.1%)	0.96	2/2209 (0.1%)
All	All	0.80	5/5209 (0.1%)	1.03	14/7048 (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
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	GLN	C-O	-6.81	1.16	1.24
1	A	421	GLN	CA-C	-6.00	1.45	1.52
2	B	645	ARG	C-O	5.54	1.30	1.24
1	A	421	GLN	N-CA	5.53	1.52	1.46
1	A	420	TYR	C-N	5.13	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	235	PRO	N-CA-C	9.04	131.10	112.47
1	A	234	PRO	CA-C-N	8.07	129.93	119.84
1	A	234	PRO	C-N-CA	8.07	129.93	119.84
1	A	37	ARG	NE-CZ-NH2	7.71	126.14	119.20
1	A	157	PRO	CB-CA-C	-6.84	104.96	111.39
1	A	420	TYR	CA-C-O	-6.19	114.28	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	GLN	O-C-N	5.99	128.26	122.03
2	B	503	ILE	N-CA-C	5.82	118.01	109.63
1	A	420	TYR	CA-C-N	5.80	128.31	120.65
1	A	420	TYR	C-N-CA	5.80	128.31	120.65
1	A	418	ARG	N-CA-C	-5.54	104.93	110.97
2	B	634	LEU	N-CA-C	5.39	117.75	109.07
1	A	418	ARG	O-C-N	-5.20	116.62	122.03
1	A	225	SER	N-CA-C	5.08	118.97	112.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	ARG	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	3480	0	3316	49	0
2	B	1607	0	1583	24	1
3	A	4	0	0	0	0
4	A	12	0	18	4	0
4	B	8	0	12	0	0
5	A	9	0	7	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	B	15	0	0	1	1
9	A	312	0	0	3	2
9	B	151	0	0	2	1
All	All	5601	0	4936	66	4

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 7.

All (66) 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:221:GLU:HG3	1:A:263:ALA:HB2	1.36	1.05
1:A:360:SER:OG	2:B:691:MET:HE2	1.55	1.04
1:A:92:GLU:OE2	2:B:683:ARG:HD3	1.62	0.99
1:A:360:SER:CB	2:B:691:MET:HE2	1.93	0.99
1:A:235:PRO:O	1:A:237:GLY:N	2.04	0.90
1:A:221:GLU:CD	1:A:263:ALA:HB3	1.96	0.90
1:A:221:GLU:OE2	1:A:263:ALA:HB3	1.72	0.89
1:A:221:GLU:CG	1:A:263:ALA:HB2	2.03	0.89
1:A:220:GLY:O	1:A:221:GLU:HG2	1.73	0.87
1:A:129:ASN:H	1:A:129:ASN:ND2	1.71	0.86
1:A:129:ASN:H	1:A:129:ASN:HD22	1.24	0.83
1:A:360:SER:OG	2:B:691:MET:CE	2.28	0.82
1:A:221:GLU:CD	1:A:263:ALA:CB	2.55	0.80
1:A:421:GLN:NE2	1:A:421:GLN:HA	2.04	0.70
2:B:604:ASP:OD2	2:B:605:PRO:HD2	1.92	0.70
1:A:221:GLU:CG	1:A:263:ALA:CB	2.70	0.69
1:A:181:GLU:HG3	1:A:334:LYS:HG2	1.75	0.68
1:A:360:SER:HB3	2:B:691:MET:HE2	1.76	0.68
2:B:580:LYS:O	2:B:581:LEU:HD12	1.94	0.68
1:A:186:PRO:CD	4:A:1451:EDO:H12	2.24	0.66
1:A:1:MET:SD	9:A:2005:HOH:O	2.53	0.66
1:A:181:GLU:HG3	1:A:334:LYS:CG	2.27	0.65
1:A:129:ASN:HD22	1:A:129:ASN:N	1.95	0.63
2:B:537:LEU:HD12	9:B:2031:HOH:O	2.00	0.62
2:B:665:ARG:NH1	8:B:1699:SO4:O1	2.35	0.56
1:A:421:GLN:HA	1:A:421:GLN:HE21	1.70	0.56
1:A:92:GLU:CD	2:B:683:ARG:HD3	2.29	0.55
1:A:360:SER:CB	2:B:691:MET:CE	2.77	0.55
1:A:186:PRO:HD2	4:A:1451:EDO:H12	1.89	0.53
1:A:221:GLU:HG3	1:A:221:GLU:O	2.08	0.53
2:B:569:ARG:NH2	9:B:2048:HOH:O	2.41	0.53
1:A:186:PRO:CG	4:A:1451:EDO:H12	2.39	0.52
1:A:3:TYR:CE2	1:A:26:LEU:HD13	2.45	0.52
2:B:531:GLN:HE21	2:B:532:GLN:NE2	2.09	0.51
2:B:532:GLN:N	2:B:532:GLN:HE21	2.07	0.51
2:B:575:SER:O	2:B:577:ARG:NH1	2.43	0.51
1:A:47:LEU:HD22	1:A:182:LEU:HD23	1.92	0.50
1:A:421:GLN:HE21	1:A:421:GLN:CA	2.26	0.49
1:A:156:ALA:HA	1:A:429:TRP:CD1	2.48	0.48
2:B:502:MET:HE3	2:B:502:MET:HA	1.94	0.48
1:A:221:GLU:CG	1:A:221:GLU:O	2.62	0.48
1:A:221:GLU:CD	1:A:263:ALA:HB2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1451:EDO:H11	2:B:570:GLU:OE2	2.15	0.47
2:B:528:SER:O	2:B:532:GLN:NE2	2.48	0.46
1:A:257:TYR:O	1:A:309:CYS:HB3	2.15	0.46
2:B:571:LEU:HD13	2:B:683:ARG:HD2	1.97	0.46
1:A:221:GLU:HG2	1:A:263:ALA:H	1.80	0.45
1:A:311:GLY:HA2	1:A:331:ILE:HG13	1.98	0.45
1:A:418:ARG:O	1:A:419:ALA:C	2.58	0.45
1:A:12:SER:HA	1:A:442:GLU:HG2	1.99	0.45
1:A:156:ALA:HA	1:A:429:TRP:NE1	2.31	0.45
1:A:220:GLY:O	1:A:221:GLU:CG	2.57	0.45
1:A:235:PRO:C	1:A:237:GLY:N	2.73	0.45
1:A:181:GLU:CG	1:A:334:LYS:HG2	2.44	0.44
1:A:181:GLU:HG3	1:A:334:LYS:HG3	1.98	0.44
1:A:253:LEU:HD13	9:A:2208:HOH:O	2.19	0.43
2:B:643:LEU:C	2:B:643:LEU:HD23	2.44	0.43
2:B:581:LEU:O	2:B:582:ASN:C	2.62	0.43
1:A:394:TYR:CG	1:A:395:GLY:N	2.87	0.42
1:A:360:SER:HA	9:A:2243:HOH:O	2.18	0.42
2:B:532:GLN:HE21	2:B:532:GLN:H	1.68	0.42
1:A:203:VAL:HG23	1:A:299:THR:HB	2.01	0.42
2:B:537:LEU:HD21	2:B:663:TRP:CE3	2.55	0.41
1:A:350:ARG:O	1:A:356:GLY:HA2	2.21	0.41
2:B:585:MET:C	2:B:585:MET:SD	3.04	0.41
1:A:446:THR:O	1:A:446:THR:HG22	2.22	0.40

All (4) 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)
9:B:2012:HOH:O	9:B:2086:HOH:O[2_665]	1.39	0.81
9:A:2271:HOH:O	9:A:2271:HOH:O[4_556]	1.66	0.54
2:B:671:ARG:NH1	8:B:1699:SO4:O3[12_555]	1.72	0.48
9:A:2269:HOH:O	9:A:2272:HOH:O[4_556]	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	445/449 (99%)	431 (97%)	11 (2%)	3 (1%)	18 6
2	B	191/194 (98%)	184 (96%)	5 (3%)	2 (1%)	12 2
All	All	636/643 (99%)	615 (97%)	16 (2%)	5 (1%)	16 4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	LYS
1	A	235	PRO
1	A	236	GLU
2	B	524	ASN
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%)	356 (97%)	11 (3%)	36 13
2	B	172/173 (99%)	160 (93%)	12 (7%)	14 2
All	All	539/542 (99%)	516 (96%)	23 (4%)	26 6

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	129	ASN
1	A	130	LYS
1	A	131	LYS
1	A	223	ILE
1	A	233	LEU
1	A	236	GLU

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	331	ILE
1	A	394	TYR
1	A	421	GLN
2	B	508	ASP
2	B	519	ILE
2	B	532	GLN
2	B	551	ARG
2	B	554	LEU
2	B	571	LEU
2	B	577	ARG
2	B	603	LEU
2	B	632	LYS
2	B	683	ARG
2	B	690	LEU
2	B	691	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	29	HIS
1	A	69	GLN
1	A	115	GLN
1	A	129	ASN
2	B	514	HIS
2	B	531	GLN
2	B	532	GLN
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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\#\|Z\| > 2$
8	SO4	B	1697	-	4,4,4	0.16	0	6,6,6	0.13	0
8	SO4	B	1698	-	4,4,4	0.23	0	6,6,6	0.30	0
6	NO	A	1453	7	0,1,1	-	-	-		
4	EDO	B	1696	-	3,3,3	0.35	0	2,2,2	0.03	0
3	FES	A	1448	1	0,4,4	-	-	-		
4	EDO	A	1449	-	3,3,3	0.33	0	2,2,2	0.36	0
4	EDO	A	1450	-	3,3,3	0.35	0	2,2,2	0.18	0
5	IND	A	1452	-	10,10,10	1.60	1 (10%)	13,13,13	3.17	8 (61%)
4	EDO	B	1695	-	3,3,3	0.36	0	2,2,2	0.26	0
4	EDO	A	1451	-	3,3,3	0.29	0	2,2,2	0.24	0
8	SO4	B	1699	-	4,4,4	0.27	0	6,6,6	0.28	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
4	EDO	B	1696	-	-	1/1/1/1	-
3	FES	A	1448	1	-	-	0/1/1/1
4	EDO	A	1449	-	-	0/1/1/1	-
4	EDO	A	1450	-	-	0/1/1/1	-
5	IND	A	1452	-	-	-	0/2/2/2
4	EDO	B	1695	-	-	1/1/1/1	-
4	EDO	A	1451	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1452	IND	C9-C8	4.26	1.46	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1452	IND	C8-C9-C3	5.29	109.75	106.62
5	A	1452	IND	C7-C8-C9	-4.98	117.85	122.17
5	A	1452	IND	C7-C8-N1	4.36	138.06	130.79
5	A	1452	IND	C9-C8-N1	-4.12	104.09	107.62
5	A	1452	IND	C8-N1-C2	3.38	111.62	108.82
5	A	1452	IND	C4-C9-C8	3.31	122.65	119.25
5	A	1452	IND	C4-C9-C3	-2.66	127.60	135.08
5	A	1452	IND	C5-C4-C9	-2.39	117.39	121.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1451	EDO	O1-C1-C2-O2
4	B	1696	EDO	O1-C1-C2-O2
4	B	1695	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1451	EDO	4	0
8	B	1699	SO4	1	1

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	447/449 (99%)	0.47	39 (8%)	16	17	24, 31, 49, 64	0
2	B	193/194 (99%)	0.45	11 (5%)	29	33	24, 30, 48, 59	0
All	All	640/643 (99%)	0.46	50 (7%)	19	22	24, 30, 49, 64	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	THR	7.3
1	A	221	GLU	5.1
1	A	228	ALA	4.3
1	A	129	ASN	4.2
1	A	233	LEU	4.1
2	B	525	CYS	4.0
1	A	224	PHE	3.8
2	B	629	VAL	3.7
1	A	240	LEU	3.7
2	B	523	PHE	3.7
1	A	235	PRO	3.7
1	A	446	THR	3.6
1	A	236	GLU	3.5
2	B	577	ARG	3.4
2	B	503	ILE	3.3
1	A	232	ALA	3.3
1	A	234	PRO	3.3
1	A	408	ILE	3.2
1	A	211	TRP	2.9
2	B	502	MET	2.9
1	A	124	TYR	2.9
1	A	125	GLY	2.9
1	A	253	LEU	2.9
1	A	203	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	223	ILE	2.8
1	A	130	LYS	2.8
1	A	227	LEU	2.7
1	A	394	TYR	2.7
2	B	569	ARG	2.6
1	A	226	SER	2.6
1	A	283	GLU	2.6
2	B	532	GLN	2.5
1	A	3	TYR	2.5
1	A	229	GLY	2.5
1	A	231	ALA	2.4
1	A	225	SER	2.4
1	A	282	LYS	2.3
1	A	363	ASN	2.3
1	A	127	SER	2.3
1	A	132	CYS	2.1
1	A	1	MET	2.1
1	A	260	VAL	2.1
2	B	526	HIS	2.1
1	A	262	SER	2.1
1	A	207	TYR	2.1
2	B	575	SER	2.0
1	A	204	GLY	2.0
1	A	119	PHE	2.0
2	B	519	ILE	2.0
1	A	445	LYS	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
5	IND	A	1452	9/9	0.75	0.18	48,49,50,50	0
4	EDO	B	1696	4/4	0.78	0.18	52,52,53,54	0
4	EDO	A	1451	4/4	0.81	0.14	38,44,44,45	0
6	NO	A	1453	2/2	0.81	0.23	37,37,37,45	0
8	SO4	B	1697	5/5	0.87	0.10	51,51,53,54	0
8	SO4	B	1699	5/5	0.89	0.12	53,54,55,55	5
4	EDO	B	1695	4/4	0.92	0.11	32,33,33,34	0
4	EDO	A	1450	4/4	0.92	0.10	28,35,37,38	0
8	SO4	B	1698	5/5	0.95	0.07	40,40,45,47	0
7	FE	A	1454	1/1	0.95	0.10	53,53,53,53	0
4	EDO	A	1449	4/4	0.97	0.06	26,27,29,30	0
3	FES	A	1448	4/4	0.99	0.03	27,29,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.