Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2023 – 09:57 PM EST

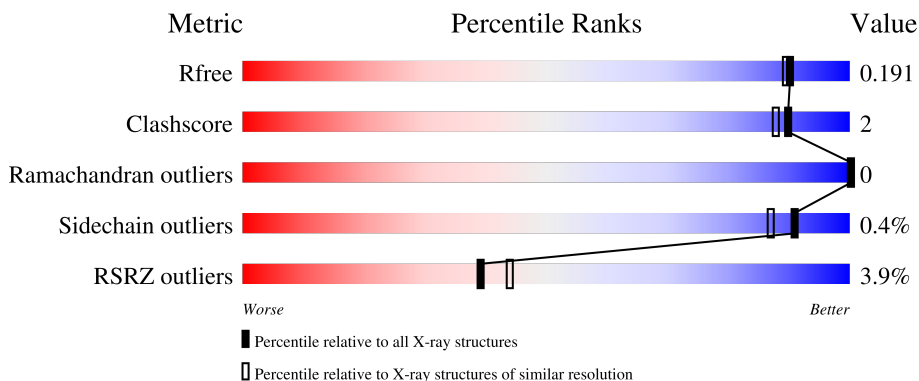|		
PDB ID	:	4HW6
Title	:	Crystal structure of an auxiliary nutrient binding protein (BACOVA_00264) from Bacteroides ovatus ATCC 8483 at 1.70 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2012-11-07
Resolution	:	1.70 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
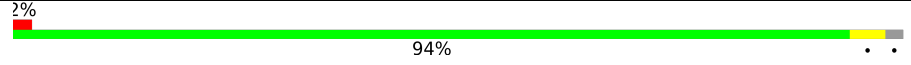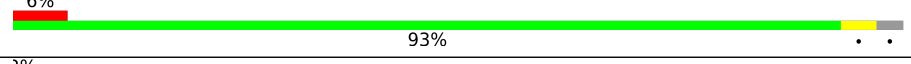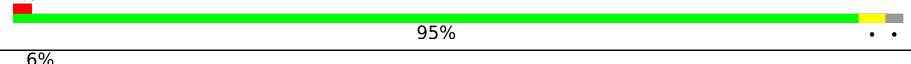*X-RAY DIFFRACTION*
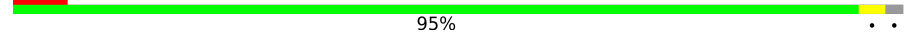
The reported resolution of this entry is 1.70 Å.

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	Percentile Ranks	Value
Rfree		0.191
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.4%
RSRZ outliers		3.9%

Worse   *Better*

▐ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	433	2% ... 94%
1	B	433	6% ... 93%
1	C	433	2% ... 95%
1	D	433	6% ... 95%

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
2	IOD	B	504	-	-	X	-
2	IOD	D	502	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15800 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 hypothetical protein, IPT/TIG domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	Se	0	13	0
			3435	2174	586	652	13	10			
1	B	422	Total	C	N	O	S	Se	0	13	0
			3415	2166	580	646	13	10			
1	C	424	Total	C	N	O	S	Se	0	13	0
			3433	2178	580	651	13	11			
1	D	424	Total	C	N	O	S	Se	0	9	0
			3425	2166	582	653	13	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A7LR39
B	0	GLY	-	expression tag	UNP A7LR39
C	0	GLY	-	expression tag	UNP A7LR39
D	0	GLY	-	expression tag	UNP A7LR39

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	I	0	0
			1	1		
2	B	5	Total	I	0	0
			5	5		
2	C	4	Total	I	0	0
			4	4		
2	D	2	Total	I	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2
OH

C1

C2

HO

O1

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

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W O R L D W I D E
PDB
PROTEIN DATA BANK

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	452	Total 463	O 463	0	10
5	B	552	Total 561	O 561	0	9
5	C	518	Total 525	O 525	0	7
5	D	451	Total 461	O 461	0	10

3 Residue-property plots ⓘ

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: hypothetical protein, IPT/TIG domain protein
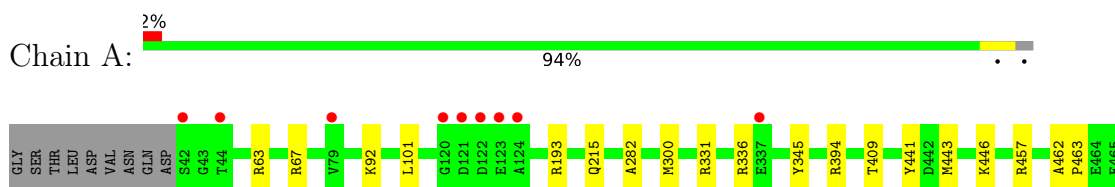
Chain A:

• Molecule 1: hypothetical protein, IPT/TIG domain protein

Chain B:

• Molecule 1: hypothetical protein, IPT/TIG domain protein

Chain C:

• Molecule 1: hypothetical protein, IPT/TIG domain protein

Chain D:
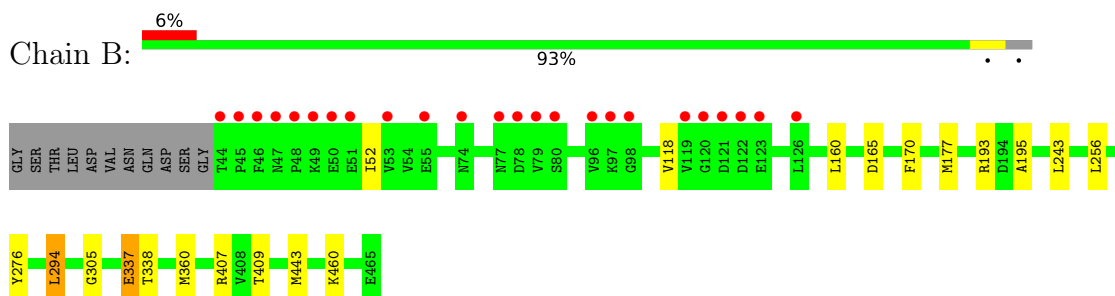
4 Data and refinement statistics ⓘ

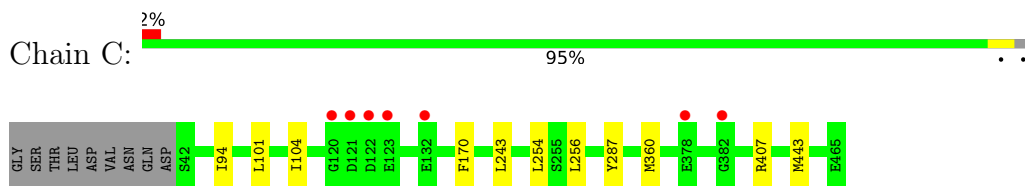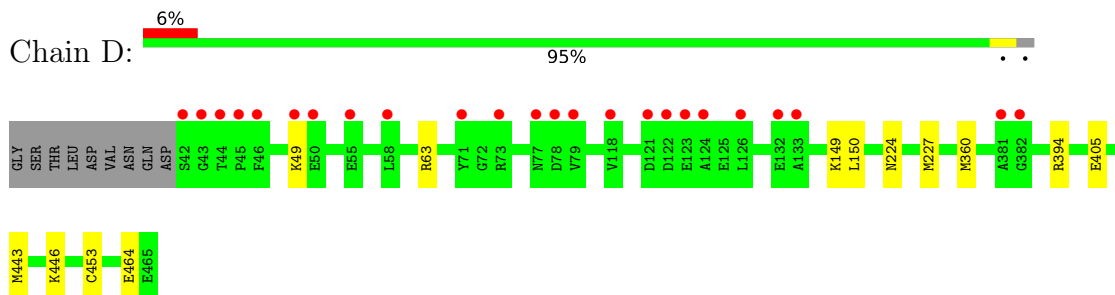| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.29Å 81.55Å 128.53Å 90.00° 108.60° 90.00°	Depositor
Resolution (Å)	29.89 – 1.70 29.89 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.89-1.70) 99.9 (29.89-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.149 , 0.179 0.162 , 0.191	Depositor DCC
R_{free} test set	11237 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15800	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CL, EDO, IOD

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	0.50	0/3553	0.72	4/4804 (0.1%)
1	B	0.50	0/3533	0.71	2/4779 (0.0%)
1	C	0.45	0/3552	0.66	0/4801
1	D	0.46	0/3534	0.69	3/4777 (0.1%)
All	All	0.48	0/14172	0.69	9/19161 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	227	MSE	CG-SE-CE	-6.30	85.04	98.90
1	D	394	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	394	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	457	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	457	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	165[A]	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	165[B]	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	394	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	336	ARG	CG-CD-NE	-5.10	101.09	111.80

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	3435	0	3284	12	0
1	B	3415	0	3266	15	0
1	C	3433	0	3283	10	0
1	D	3425	0	3267	7	0
2	A	1	0	0	0	0
2	B	5	0	0	4	0
2	C	4	0	0	1	0
2	D	2	0	0	3	0
3	A	8	0	12	0	0
3	B	28	0	42	0	0
3	C	8	0	12	0	0
3	D	16	0	24	1	0
4	A	4	0	0	1	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	463	0	0	2	0
5	B	561	0	0	4	0
5	C	525	0	0	1	0
5	D	461	0	0	5	0
All	All	15800	0	13190	49	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 2.

All (49) 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:D:502:IOD:I	5:D:1012:HOH:O	2.27	1.23
4:A:507:CL:CL	5:A:912[B]:HOH:O	2.33	0.83
1:A:443[B]:MSE:HE2	1:A:446:LYS:NZ	2.04	0.73
1:D:63[A]:ARG:NH1	1:D:464[A]:GLU:OE2	2.18	0.70
1:A:443[B]:MSE:HE2	1:A:446:LYS:HZ3	1.56	0.68
2:D:502:IOD:I	5:D:702:HOH:O	2.83	0.66
2:B:505:IOD:I	5:B:787:HOH:O	2.85	0.65
1:D:453[B]:CYS:SG	5:D:1045:HOH:O	2.57	0.60
1:B:337:GLU:HG2	1:B:338:THR:HG23	1.83	0.59
1:C:256:LEU:HG	1:C:287[B]:TYR:CE2	2.38	0.59
1:D:360:MSE:HE1	1:D:405:GLU:CD	2.23	0.59
1:A:443[B]:MSE:CE	1:A:446:LYS:NZ	2.69	0.55
1:A:443[B]:MSE:CE	1:A:446:LYS:HZ2	2.21	0.54
1:B:460:LYS:NZ	5:B:1141:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:MSE:CE	1:C:407:ARG:CZ	2.89	0.50
1:A:282:ALA:O	1:A:300[A]:MSE:HE3	2.11	0.50
1:B:170:PHE:HA	2:B:504:IOD:I	2.83	0.49
1:C:170:PHE:HA	2:C:504:IOD:I	2.82	0.49
1:C:360:MSE:HE2	1:C:407:ARG:CZ	2.42	0.49
1:C:360:MSE:CE	1:C:407:ARG:NH2	2.75	0.49
1:D:149:LYS:HD2	5:D:804:HOH:O	2.13	0.48
2:D:501:IOD:I	5:D:1006:HOH:O	2.91	0.48
1:B:276:TYR:OH	1:B:294[A]:LEU:HD21	2.13	0.47
1:B:337:GLU:CG	1:B:338:THR:HG23	2.45	0.47
1:D:224[A]:ASN:HB2	3:D:503:EDO:H22	1.96	0.47
1:C:243[B]:LEU:CD1	1:C:256:LEU:HD13	2.45	0.47
1:A:331[B]:ARG:HD2	1:A:345:TYR:OH	2.16	0.46
1:C:243[A]:LEU:HD22	1:C:254:LEU:HD12	1.97	0.46
1:C:443[B]:MSE:HE1	5:C:1027:HOH:O	2.16	0.46
1:C:94:ILE:HD11	1:C:104:ILE:HD11	1.97	0.45
1:D:443[A]:MSE:SE	1:D:446:LYS:NZ	3.01	0.44
1:A:443[B]:MSE:HE1	1:A:446:LYS:HZ2	1.82	0.44
1:B:360:MSE:CE	1:B:407:ARG:CZ	2.95	0.44
1:A:193:ARG:HE	1:A:215:GLN:NE2	2.16	0.43
1:B:177:MSE:HE3	1:B:177:MSE:HB2	1.96	0.43
1:B:243[B]:LEU:HD22	1:B:256:LEU:HD21	2.00	0.43
1:B:409[B]:THR:HG23	5:B:1012:HOH:O	2.18	0.42
1:A:441:TYR:HE2	1:A:443[B]:MSE:HE3	1.84	0.42
1:C:101:LEU:C	1:C:101:LEU:HD12	2.41	0.42
1:B:160:LEU:N	1:B:160:LEU:HD23	2.35	0.42
1:B:195:ALA:HB3	2:B:504:IOD:I	2.90	0.42
1:B:193:ARG:HD3	2:B:502:IOD:I	2.90	0.41
1:D:149:LYS:C	1:D:150:LEU:HD12	2.41	0.41
1:A:409:THR:HG23	5:A:710:HOH:O	2.19	0.41
1:A:101:LEU:C	1:A:101:LEU:HD12	2.42	0.41
1:B:52:ILE:HD11	1:B:118:VAL:HG23	2.03	0.40
1:B:305:GLY:O	5:B:861:HOH:O	2.22	0.40
1:A:462:ALA:HB1	1:A:463:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

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	435/433 (100%)	421 (97%)	14 (3%)	0	100	100
1	B	433/433 (100%)	422 (98%)	11 (2%)	0	100	100
1	C	435/433 (100%)	424 (98%)	11 (2%)	0	100	100
1	D	432/433 (100%)	419 (97%)	13 (3%)	0	100	100
All	All	1735/1732 (100%)	1686 (97%)	49 (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	372/361 (103%)	368 (99%)	4 (1%)	73	63
1	B	369/361 (102%)	366 (99%)	3 (1%)	81	74
1	C	371/361 (103%)	371 (100%)	0	100	100
1	D	371/361 (103%)	370 (100%)	1 (0%)	92	89
All	All	1483/1444 (103%)	1475 (100%)	8 (0%)	91	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	67[A]	ARG

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Mol	Chain	Res	Type
1	A	67[B]	ARG
1	A	92	LYS
1	B	294[A]	LEU
1	B	294[B]	LEU
1	B	337	GLU
1	D	49	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	C	350	GLN
1	D	138	GLN
1	D	350	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 ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 22 are monoatomic - leaving 15 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	509	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	B	512	-	3,3,3	0.75	0	2,2,2	0.31	0
3	EDO	D	504	-	3,3,3	0.48	0	2,2,2	0.24	0
3	EDO	D	505	-	3,3,3	0.50	0	2,2,2	0.21	0
3	EDO	B	510	-	3,3,3	0.52	0	2,2,2	0.35	0
3	EDO	B	508	-	3,3,3	0.40	0	2,2,2	0.53	0
3	EDO	B	506	-	3,3,3	0.57	0	2,2,2	0.11	0
3	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.22	0
3	EDO	C	506	-	3,3,3	0.45	0	2,2,2	0.10	0
3	EDO	D	506	-	3,3,3	0.44	0	2,2,2	0.21	0
3	EDO	C	505	-	3,3,3	0.29	0	2,2,2	0.78	0
3	EDO	D	503	-	3,3,3	0.40	0	2,2,2	0.67	0
3	EDO	A	503	-	3,3,3	0.56	0	2,2,2	0.29	0
3	EDO	B	507	-	3,3,3	0.34	0	2,2,2	0.45	0
3	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.24	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	B	509	-	-	0/1/1/1	-
3	EDO	B	512	-	-	0/1/1/1	-
3	EDO	D	504	-	-	1/1/1/1	-
3	EDO	D	505	-	-	1/1/1/1	-
3	EDO	B	510	-	-	0/1/1/1	-
3	EDO	B	508	-	-	1/1/1/1	-
3	EDO	B	506	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	C	506	-	-	0/1/1/1	-
3	EDO	D	506	-	-	0/1/1/1	-
3	EDO	C	505	-	-	1/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
3	EDO	B	511	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	508	EDO	O1-C1-C2-O2
3	D	503	EDO	O1-C1-C2-O2
3	C	505	EDO	O1-C1-C2-O2
3	B	506	EDO	O1-C1-C2-O2
3	D	504	EDO	O1-C1-C2-O2
3	D	505	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	416/433 (96%)	-0.27	9 (2%)	62	66	12, 20, 47, 86	0
1	B	414/433 (95%)	-0.10	24 (5%)	23	25	12, 19, 71, 109	0
1	C	416/433 (96%)	-0.24	7 (1%)	70	74	15, 23, 48, 86	0
1	D	416/433 (96%)	-0.02	24 (5%)	23	25	14, 22, 81, 126	0
All	All	1662/1732 (95%)	-0.16	64 (3%)	39	44	12, 21, 64, 126	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	SER	6.8
1	B	45	PRO	6.4
1	B	121	ASP	5.9
1	D	121	ASP	5.9
1	D	49	LYS	5.7
1	B	122	ASP	5.5
1	D	45	PRO	5.5
1	D	122	ASP	5.1
1	D	46	PHE	4.9
1	B	120	GLY	4.8
1	D	43	GLY	4.6
1	B	79[A]	VAL	4.5
1	B	48	PRO	4.5
1	A	120	GLY	4.2
1	D	132	GLU	4.1
1	D	133	ALA	4.1
1	D	58	LEU	4.0
1	B	46	PHE	3.9
1	B	44	THR	3.9
1	D	50	GLU	3.8
1	C	120	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	121	ASP	3.7
1	A	42	SER	3.7
1	A	121	ASP	3.5
1	B	96	VAL	3.4
1	B	123	GLU	3.4
1	A	122	ASP	3.4
1	D	55	GLU	3.4
1	A	124	ALA	3.3
1	D	78	ASP	3.1
1	B	53	VAL	3.1
1	B	47	ASN	3.1
1	D	44	THR	3.1
1	D	118	VAL	3.0
1	D	126	LEU	3.0
1	B	77	ASN	2.9
1	C	122	ASP	2.9
1	A	123	GLU	2.8
1	D	123	GLU	2.8
1	B	78	ASP	2.8
1	B	80	SER	2.7
1	B	49	LYS	2.7
1	B	98	GLY	2.6
1	A	79[A]	VAL	2.5
1	C	132	GLU	2.5
1	D	381	ALA	2.5
1	D	124	ALA	2.5
1	B	51	GLU	2.5
1	B	126	LEU	2.5
1	D	382	GLY	2.5
1	D	77	ASN	2.4
1	C	382	GLY	2.4
1	D	71	TYR	2.3
1	B	97	LYS	2.3
1	A	44	THR	2.3
1	D	73	ARG	2.3
1	A	337[A]	GLU	2.3
1	C	123	GLU	2.2
1	B	55	GLU	2.2
1	C	378	GLU	2.2
1	B	119	VAL	2.1
1	D	79	VAL	2.1
1	B	50	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	74	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	EDO	B	512	4/4	0.77	0.20	31,36,42,42	0
3	EDO	D	505	4/4	0.81	0.15	44,46,46,53	0
3	EDO	B	511	4/4	0.86	0.14	35,36,44,50	0
3	EDO	D	503	4/4	0.87	0.14	19,25,42,43	0
3	EDO	B	506	4/4	0.89	0.08	29,31,31,36	0
3	EDO	D	504	4/4	0.90	0.10	32,36,37,46	0
2	IOD	C	502	1/1	0.91	0.08	29,29,29,29	1
3	EDO	D	506	4/4	0.91	0.14	42,46,47,62	0
3	EDO	B	507	4/4	0.92	0.15	23,26,38,49	0
3	EDO	B	510	4/4	0.92	0.13	25,31,37,39	0
3	EDO	B	508	4/4	0.93	0.15	20,29,35,39	0
3	EDO	C	505	4/4	0.93	0.11	23,28,41,50	0
3	EDO	A	503	4/4	0.94	0.14	27,28,31,32	0
3	EDO	A	502	4/4	0.94	0.07	27,31,31,38	0
3	EDO	B	509	4/4	0.95	0.12	28,34,37,47	0
3	EDO	C	506	4/4	0.95	0.06	30,35,37,41	0
2	IOD	A	501	1/1	0.95	0.04	47,47,47,47	1
2	IOD	C	503	1/1	0.97	0.05	28,28,28,28	1
4	CL	A	504	1/1	0.97	0.07	33,33,33,33	0
4	CL	D	507	1/1	0.97	0.04	35,35,35,35	0
4	CL	C	507	1/1	0.98	0.05	32,32,32,32	0
2	IOD	B	505	1/1	0.99	0.07	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IOD	B	501	1/1	0.99	0.06	22,22,22,22	1
2	IOD	B	503	1/1	0.99	0.05	23,23,23,23	1
2	IOD	C	504	1/1	0.99	0.04	20,20,20,20	1
4	CL	A	505	1/1	0.99	0.07	26,26,26,26	0
4	CL	A	507	1/1	0.99	0.05	23,23,23,23	0
4	CL	B	513	1/1	0.99	0.03	26,26,26,26	0
4	CL	B	514	1/1	0.99	0.07	16,16,16,16	0
4	CL	B	515	1/1	0.99	0.03	36,36,36,36	0
2	IOD	D	501	1/1	0.99	0.06	20,20,20,20	1
2	IOD	D	502	1/1	0.99	0.07	29,29,29,29	1
2	IOD	B	504	1/1	1.00	0.05	17,17,17,17	1
4	CL	A	506	1/1	1.00	0.04	18,18,18,18	0
2	IOD	B	502	1/1	1.00	0.04	21,21,21,21	1
2	IOD	C	501	1/1	1.00	0.06	20,20,20,20	1
4	CL	D	508	1/1	1.00	0.06	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.