



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2018 – 08:18 am GMT

PDB ID : 1OSB
Title : Conjugative Relaxase TrwC in complex with OriT Dna. Metal-free structure.
Authors : Guasch, A.; Lucas, M.; Moncalian, G.; Cabezas, M.; Perez-Luque, R.; Gomis-Ruth, F.X.; de la Cruz, F.; Coll, M.
Deposited on : 2003-03-19
Resolution : 2.65 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

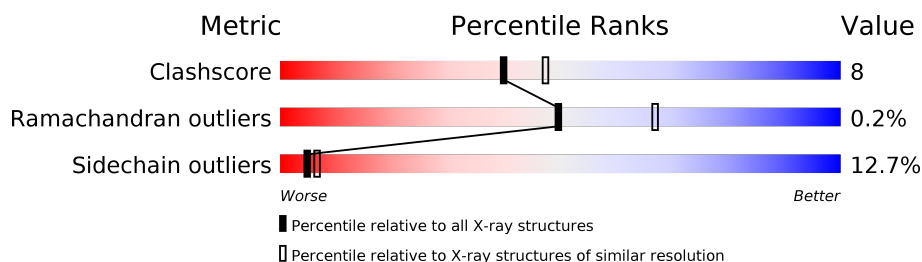
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
Clashscore	122078	1151 (2.68-2.64)
Ramachandran outliers	120005	1133 (2.68-2.64)
Sidechain outliers	119972	1133 (2.68-2.64)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	25	
1	D	25	
2	A	293	
2	C	293	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5802 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 DNA chain called Dna oligonucleotide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	25	Total	C	N	O	P	0	0	0
			506	238	95	149	24			
1	D	25	Total	C	N	O	P	0	0	0
			506	238	95	149	24			

- Molecule 2 is a protein called TrwC protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	287	Total	C	N	O	S	0	0	0
			2260	1391	429	436	4			
2	C	282	Total	C	N	O	S	0	0	0
			2228	1375	424	425	4			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	16	Total O 16 16	0	0
4	D	9	Total O 9 9	0	0
4	A	140	Total O 140 140	0	0
4	C	92	Total O 92 92	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

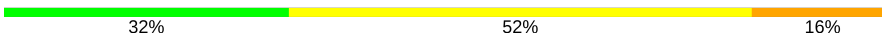
Note EDS was not executed.

• Molecule 1: Dna oligonucleotide

Chain B: 



• Molecule 1: Dna oligonucleotide

Chain D: 



• Molecule 2: TrwC protein

Chain A: 



• Molecule 2: TrwC protein

Chain C: 





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	147.78Å 147.78Å 78.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.65	Depositor
% Data completeness (in resolution range)	2.2 (40.00-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.195 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5802	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	B	1.02	0/568	1.53	8/873 (0.9%)
1	D	0.94	0/568	1.54	12/873 (1.4%)
2	A	0.49	0/2290	0.95	24/3071 (0.8%)
2	C	0.46	0/2258	0.95	22/3029 (0.7%)
All	All	0.61	0/5684	1.11	66/7846 (0.8%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	156	ARG	NE-CZ-NH1	-11.09	114.75	120.30
2	C	156	ARG	NE-CZ-NH2	9.91	125.26	120.30
1	B	2	DC	O4'-C1'-N1	9.72	114.80	108.00
2	A	56	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	D	2	DC	O4'-C1'-N1	8.76	114.13	108.00
1	D	9	DA	O4'-C1'-N9	8.73	114.11	108.00
2	C	112	ARG	NE-CZ-NH1	-8.45	116.07	120.30
2	A	136	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	D	21	DT	O4'-C1'-N1	8.30	113.81	108.00
2	A	56	ARG	NE-CZ-NH1	-8.19	116.21	120.30
2	C	56	ARG	NE-CZ-NH2	-8.14	116.23	120.30
2	C	14	ARG	NE-CZ-NH2	8.13	124.36	120.30
2	A	116	ARG	NE-CZ-NH2	-8.11	116.25	120.30
2	C	136	ARG	NE-CZ-NH1	-8.08	116.26	120.30
2	A	156	ARG	NE-CZ-NH2	-8.07	116.26	120.30
2	C	136	ARG	NE-CZ-NH2	8.01	124.30	120.30
2	C	14	ARG	NE-CZ-NH1	-7.96	116.32	120.30
2	C	112	ARG	NE-CZ-NH2	7.93	124.27	120.30
1	B	21	DT	O4'-C1'-N1	7.69	113.38	108.00
1	B	13	DG	O4'-C1'-N9	-7.65	102.65	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	249	ASP	CB-CG-OD2	7.44	125.00	118.30
2	A	116	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	A	14	ARG	NE-CZ-NH1	7.34	123.97	120.30
2	C	56	ARG	NE-CZ-NH1	7.25	123.92	120.30
2	A	14	ARG	NE-CZ-NH2	-7.20	116.70	120.30
2	C	103	ASP	CB-CG-OD2	7.19	124.77	118.30
1	B	12	DG	O4'-C1'-N9	7.16	113.01	108.00
2	A	112	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	A	156	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	18	DT	O4'-C1'-N1	6.92	112.84	108.00
2	A	112	ARG	NE-CZ-NH1	6.89	123.75	120.30
2	C	249	ASP	CB-CG-OD2	6.86	124.48	118.30
2	A	136	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	D	25	DT	N3-C2-O2	-6.77	118.24	122.30
1	D	13	DG	O4'-C1'-N9	-6.60	103.38	108.00
2	C	116	ARG	NE-CZ-NH1	-6.45	117.08	120.30
2	C	116	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	C	246	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	D	18	DT	O4'-C1'-N1	6.13	112.29	108.00
2	C	246	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	A	246	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	A	246	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	A	51	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	6	DC	O4'-C1'-N1	5.74	112.02	108.00
1	D	9	DA	C1'-O4'-C4'	-5.74	104.36	110.10
1	D	20	DT	C5-C4-O4	-5.67	120.93	124.90
1	B	16	DC	C1'-O4'-C4'	-5.65	104.45	110.10
2	A	103	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	19	DA	P-O3'-C3'	5.53	126.33	119.70
1	D	6	DC	O4'-C1'-N1	5.50	111.85	108.00
2	A	85	ASP	CB-CG-OD2	5.45	123.20	118.30
1	D	9	DA	O4'-C1'-C2'	-5.41	101.57	105.90
2	A	216	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	16	DC	C1'-O4'-C4'	-5.40	104.70	110.10
2	C	85	ASP	CB-CG-OD2	5.33	123.10	118.30
2	A	24	ASP	CB-CG-OD2	5.31	123.08	118.30
2	A	77	ASP	CB-CG-OD2	5.29	123.07	118.30
2	C	11	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	20	DT	N3-C4-O4	5.27	123.06	119.90
2	A	32	ASP	CB-CG-OD2	5.25	123.03	118.30
2	A	220	ASP	CB-CG-OD2	5.25	123.02	118.30
2	C	216	ASP	CB-CG-OD2	5.21	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	51	ASP	CB-CG-OD2	5.19	122.97	118.30
2	C	174	ASP	CB-CG-OD2	5.04	122.84	118.30
2	A	167	LEU	CA-CB-CG	-5.02	103.75	115.30
2	C	157	ASP	CB-CG-OD2	5.01	122.81	118.30

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	B	506	0	265	13	0
1	D	506	0	265	12	0
2	A	2260	0	2249	38	0
2	C	2228	0	2228	32	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
4	A	140	0	0	5	0
4	B	16	0	0	0	0
4	C	92	0	0	4	0
4	D	9	0	0	0	0
All	All	5802	0	5007	83	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 8.

All (83) 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:C:156:ARG:NH1	2:C:270:THR:O	1.88	1.04
2:A:22:GLY:HA3	4:C:513:HOH:O	1.57	1.03
2:C:142:ASN:HD21	2:C:171:LYS:H	1.15	0.95
2:A:142:ASN:HD21	2:A:171:LYS:H	1.14	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:DT:H3	2:C:182:ASN:HD21	1.19	0.90
2:C:156:ARG:HH12	2:C:270:THR:C	1.84	0.80
2:A:274:ARG:NH1	4:A:515:HOH:O	2.15	0.79
2:C:223:HIS:CE1	4:C:731:HOH:O	2.37	0.78
1:D:18:DT:H3	2:C:182:ASN:ND2	1.86	0.72
2:C:223:HIS:CE1	4:C:732:HOH:O	2.43	0.72
2:C:154:ARG:HH22	2:C:266:ARG:CZ	2.04	0.70
1:B:11:DA:H5'	1:B:11:DA:N3	2.08	0.69
2:A:23:ALA:O	2:A:24:ASP:HB3	1.95	0.66
2:A:37:GLN:HE21	2:A:147:LYS:NZ	1.94	0.66
1:B:18:DT:H3	2:A:182:ASN:HD21	1.44	0.64
2:C:225:ASP:H	2:C:228:GLN:HE21	1.45	0.64
2:C:37:GLN:HE21	2:C:147:LYS:NZ	1.95	0.62
2:A:176:GLN:HG3	2:A:178:ARG:NH2	2.16	0.61
1:B:19:DA:H2''	1:B:20:DT:H5'	1.82	0.61
2:A:154:ARG:HH22	2:A:266:ARG:CZ	2.14	0.61
1:B:8:DG:H21	1:B:10:DA:H2	1.47	0.61
2:C:225:ASP:H	2:C:228:GLN:NE2	1.99	0.60
2:A:39:LYS:HG2	4:A:536:HOH:O	2.02	0.59
2:A:168:ASN:ND2	2:A:180:LEU:H	2.00	0.59
2:C:176:GLN:HG3	2:C:178:ARG:NH2	2.18	0.59
1:D:15:DG:O6	2:C:128:ARG:NH2	2.36	0.58
2:A:225:ASP:H	2:A:228:GLN:HE21	1.52	0.57
2:A:171:LYS:HE2	4:A:592:HOH:O	2.03	0.57
1:B:23:DT:OP1	2:A:226:ARG:NH2	2.37	0.57
2:A:225:ASP:H	2:A:228:GLN:NE2	2.02	0.56
2:C:223:HIS:ND1	4:C:731:HOH:O	2.33	0.56
1:D:19:DA:H2''	1:D:20:DT:H5'	1.87	0.56
2:C:156:ARG:NH2	2:C:269:LYS:HB3	2.23	0.54
1:B:2:DC:H2''	1:B:3:DG:H5'	1.89	0.53
2:C:174:ASP:OD1	2:C:176:GLN:HB2	2.09	0.53
2:A:37:GLN:HE21	2:A:147:LYS:HZ3	1.55	0.52
2:A:100:VAL:O	2:A:278:ARG:NH2	2.42	0.52
2:C:182:ASN:HD22	2:C:182:ASN:C	2.12	0.52
2:A:182:ASN:HD22	2:A:182:ASN:C	2.13	0.52
2:C:37:GLN:NE2	2:C:147:LYS:NZ	2.58	0.52
2:A:156:ARG:NH1	2:A:270:THR:O	2.42	0.52
1:B:23:DT:P	2:A:226:ARG:HH22	2.33	0.51
2:A:274:ARG:HD2	4:A:754:HOH:O	2.09	0.51
1:B:15:DG:H5'	2:A:74:THR:HG23	1.92	0.51
1:D:22:DG:C2	2:C:1:MET:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:DG:H3'	2:C:130:LYS:O	2.11	0.51
2:C:168:ASN:ND2	2:C:180:LEU:H	2.09	0.50
1:B:2:DC:H2''	1:B:3:DG:C5'	2.42	0.50
1:D:23:DT:OP1	2:C:226:ARG:NH2	2.43	0.50
2:A:37:GLN:NE2	2:A:147:LYS:NZ	2.58	0.49
1:D:10:DA:N3	1:D:10:DA:H2'	2.26	0.49
1:B:22:DG:C2	2:A:1:MET:HG2	2.47	0.49
2:A:37:GLN:HE22	2:A:115:ALA:HA	1.78	0.49
2:C:154:ARG:NH2	2:C:266:ARG:CZ	2.74	0.49
1:D:2:DC:H2''	1:D:3:DG:H5'	1.95	0.49
2:A:173:SER:HB3	4:A:757:HOH:O	2.13	0.49
2:A:59:LEU:HD22	2:A:82:ILE:HD12	1.95	0.48
1:B:18:DT:H3	2:A:182:ASN:ND2	2.10	0.48
2:C:37:GLN:HE21	2:C:147:LYS:HZ3	1.60	0.48
2:C:59:LEU:HD22	2:C:82:ILE:HD12	1.96	0.48
2:C:158:PRO:HG3	2:C:281:TRP:CD2	2.49	0.48
2:A:101:ALA:HB2	2:A:292:PHE:CG	2.50	0.47
2:A:110:HIS:ND1	2:A:196:TYR:OH	2.45	0.47
1:B:12:DG:H2''	1:B:13:DG:O5'	2.15	0.47
2:C:4:HIS:HA	2:C:85:ASP:O	2.14	0.47
1:D:2:DC:H2''	1:D:3:DG:C5'	2.46	0.46
1:D:8:DG:H21	1:D:10:DA:H2	1.62	0.45
2:C:37:GLN:HE22	2:C:115:ALA:HA	1.80	0.45
2:A:99:LEU:O	2:A:278:ARG:HD3	2.18	0.44
2:A:4:HIS:HA	2:A:85:ASP:O	2.18	0.44
2:A:124:ARG:HB3	2:A:184:GLU:HB2	1.99	0.43
2:A:138:GLU:OE2	2:A:173:SER:HB2	2.17	0.43
2:C:37:GLN:NE2	2:C:147:LYS:HZ2	2.16	0.43
2:C:156:ARG:HH11	2:C:272:VAL:HB	1.84	0.43
1:D:12:DG:H2''	1:D:13:DG:O5'	2.19	0.42
2:C:201:ALA:O	2:C:205:GLN:HG3	2.20	0.42
1:B:17:DG:H2''	1:B:18:DT:O5'	2.21	0.41
2:A:154:ARG:NH2	2:A:266:ARG:CZ	2.81	0.41
2:A:172:ARG:CZ	2:A:178:ARG:HD3	2.50	0.41
2:A:156:ARG:NH2	2:A:269:LYS:HB3	2.36	0.41
2:C:124:ARG:HB3	2:C:184:GLU:HB2	2.03	0.41
2:A:182:ASN:HD22	2:A:183:ASP:N	2.18	0.40
2:A:249:ASP:HA	2:A:250:PRO:HD2	1.94	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	
2	A	283/293 (97%)	274 (97%)	8 (3%)	1 (0%)	36	52
2	C	278/293 (95%)	269 (97%)	9 (3%)	0	100	100
All	All	561/586 (96%)	543 (97%)	17 (3%)	1 (0%)	49	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	21	ASP

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	
2	A	229/234 (98%)	199 (87%)	30 (13%)	4	6
2	C	226/234 (97%)	198 (88%)	28 (12%)	5	7
All	All	455/468 (97%)	397 (87%)	58 (13%)	5	6

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	LEU
2	A	7	LEU
2	A	12	ILE
2	A	14	ARG
2	A	20	GLU

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Mol	Chain	Res	Type
2	A	21	ASP
2	A	24	ASP
2	A	32	ASP
2	A	35	GLU
2	A	43	GLU
2	A	96	LEU
2	A	134	LYS
2	A	154	ARG
2	A	178	ARG
2	A	182	ASN
2	A	190	ARG
2	A	206	LYS
2	A	215	LYS
2	A	223	HIS
2	A	226	ARG
2	A	246	ARG
2	A	248	LEU
2	A	253	VAL
2	A	255	LEU
2	A	259	GLN
2	A	269	LYS
2	A	270	THR
2	A	271	SER
2	A	274	ARG
2	A	278	ARG
2	C	2	LEU
2	C	7	LEU
2	C	12	ILE
2	C	20	GLU
2	C	35	GLU
2	C	43	GLU
2	C	52	SER
2	C	96	LEU
2	C	131	ILE
2	C	132	GLN
2	C	154	ARG
2	C	176	GLN
2	C	178	ARG
2	C	182	ASN
2	C	190	ARG
2	C	206	LYS
2	C	215	LYS

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Mol	Chain	Res	Type
2	C	223	HIS
2	C	226	ARG
2	C	246	ARG
2	C	253	VAL
2	C	255	LEU
2	C	259	GLN
2	C	269	LYS
2	C	270	THR
2	C	271	SER
2	C	274	ARG
2	C	278	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	37	GLN
2	A	62	ASN
2	A	67	HIS
2	A	132	GLN
2	A	142	ASN
2	A	168	ASN
2	A	182	ASN
2	A	197	ASN
2	A	210	GLN
2	A	228	GLN
2	A	257	GLN
2	C	37	GLN
2	C	62	ASN
2	C	142	ASN
2	C	168	ASN
2	C	182	ASN
2	C	197	ASN
2	C	210	GLN
2	C	228	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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	SO4	A	803	-	4,4,4	0.11	0	6,6,6	0.31	0
3	SO4	A	804	-	4,4,4	0.19	0	6,6,6	0.11	0
3	SO4	A	805	-	4,4,4	0.28	0	6,6,6	0.12	0
3	SO4	B	801	-	4,4,4	0.10	0	6,6,6	0.31	0
3	SO4	B	802	-	4,4,4	0.14	0	6,6,6	0.29	0
3	SO4	C	806	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	C	808	-	4,4,4	0.17	0	6,6,6	0.22	0
3	SO4	C	809	-	4,4,4	0.19	0	6,6,6	0.39	0
3	SO4	D	807	-	4,4,4	0.21	0	6,6,6	0.16	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	SO4	A	803	-	-	0/0/0/0	0/0/0/0
3	SO4	A	804	-	-	0/0/0/0	0/0/0/0
3	SO4	A	805	-	-	0/0/0/0	0/0/0/0
3	SO4	B	801	-	-	0/0/0/0	0/0/0/0
3	SO4	B	802	-	-	0/0/0/0	0/0/0/0
3	SO4	C	806	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	808	-	-	0/0/0/0	0/0/0/0
3	SO4	C	809	-	-	0/0/0/0	0/0/0/0
3	SO4	D	807	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.