



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:37 AM GMT

PDB ID : 2DPP
Title : Crystal structure of thermostable Bacillus sp. RAPc8 nitrile hydratase
Authors : Tsekoa, T.L.; Tastan-Bishop, A.O.; Cameron, R.A.; Sewell, B.T.; Sayed, M.F.; Cowan, D.A.
Deposited on : 2006-05-12
Resolution : 2.52 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

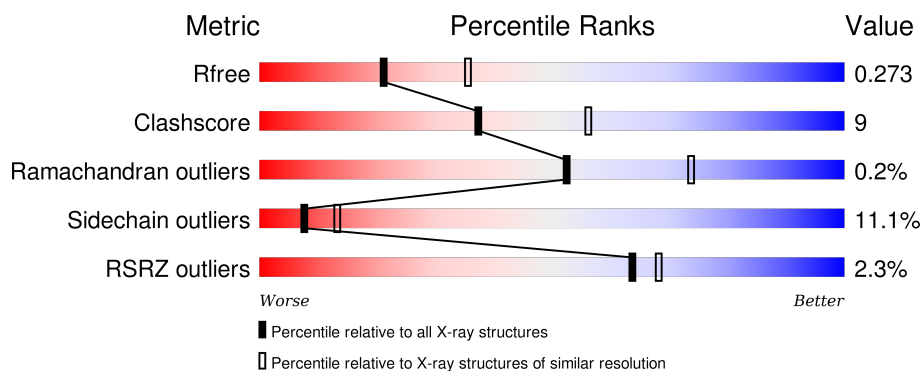
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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 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.

Mol	Chain	Length	Quality of chain
1	A	216	 73% 17% •• 6%
2	B	229	 4% 72% 23% •••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3692 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 Nitrile hydratase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1631	1039	284	301	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	CSD	CYS	MODIFIED RESIDUE	UNP Q84FS5
A	121	CSO	CYS	MODIFIED RESIDUE	UNP Q84FS5

- Molecule 2 is a protein called Nitrile hydratase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1857	1193	313	343	8			

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Co	0	0
			1	1		

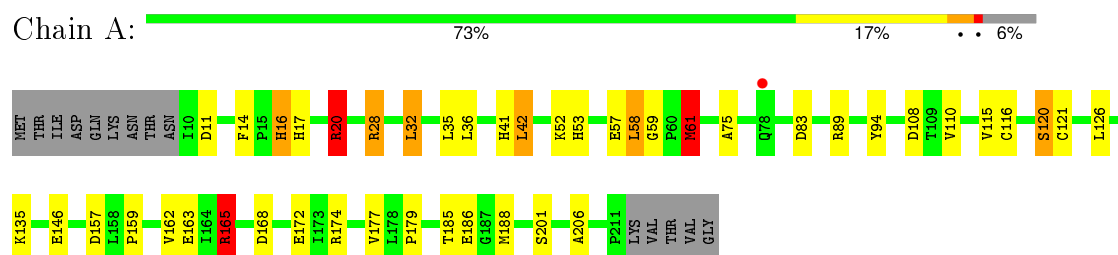
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	116	Total	O	0	0
			116	116		

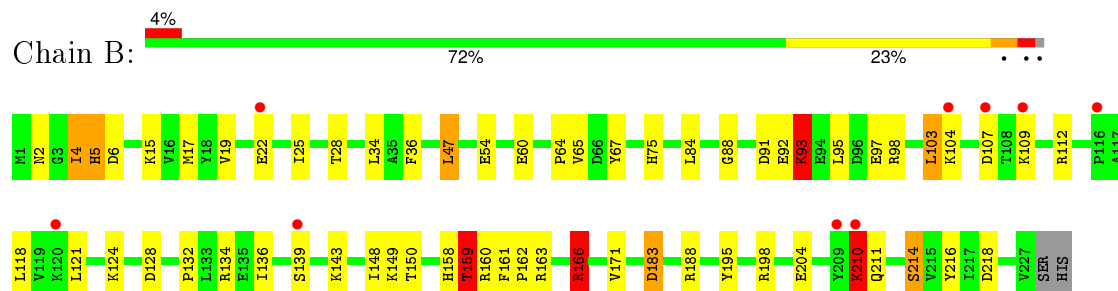
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Nitrile hydratase alpha subunit



• Molecule 2: Nitrile hydratase beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.62Å 106.62Å 83.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.52 19.80 – 2.52	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.52) 99.9 (19.80-2.52)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.279 0.195 , 0.273	Depositor DCC
R_{free} test set	831 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 16682 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3692	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 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CSD, CSO, CO

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	1.26	6/1660 (0.4%)	1.14	12/2256 (0.5%)
2	B	1.29	4/1907 (0.2%)	1.18	14/2577 (0.5%)
All	All	1.27	10/3567 (0.3%)	1.16	26/4833 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	LYS	CD-CE	8.10	1.71	1.51
2	B	210	LYS	CB-CG	6.54	1.70	1.52
2	B	210	LYS	CE-NZ	6.21	1.64	1.49
1	A	75	ALA	CA-CB	6.21	1.65	1.52
1	A	146	GLU	CG-CD	5.72	1.60	1.51
1	A	163	GLU	CD-OE2	5.46	1.31	1.25
1	A	61	MET	CG-SD	5.30	1.95	1.81
1	A	146	GLU	CD-OE1	5.29	1.31	1.25
2	B	93	LYS	CE-NZ	5.20	1.62	1.49
1	A	110	VAL	CB-CG2	5.08	1.63	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	166	ARG	NE-CZ-NH1	-11.30	114.65	120.30
1	A	165	ARG	NE-CZ-NH2	10.19	125.39	120.30
2	B	166	ARG	NE-CZ-NH2	8.87	124.73	120.30
1	A	165	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	A	157	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	28	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	A	28	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	B	163	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	83	ASP	CB-CG-OD2	6.75	124.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ARG	NE-CZ-NH1	-6.66	116.97	120.30
2	B	188	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	20	ARG	NE-CZ-NH2	6.22	123.41	120.30
2	B	159	THR	CB-CA-C	-6.16	94.97	111.60
2	B	188	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	B	134	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	B	198	ARG	NE-CZ-NH1	-5.81	117.40	120.30
2	B	98	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	A	32	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	108	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	168	ASP	CB-CG-OD1	5.58	123.32	118.30
2	B	218	ASP	CB-CG-OD2	5.50	123.25	118.30
2	B	166	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	11	ASP	CB-CG-OD1	5.27	123.04	118.30
2	B	134	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	B	47	LEU	CA-CB-CG	5.17	127.19	115.30
2	B	166	ARG	CG-CD-NE	-5.05	101.19	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	1631	0	1611	24	0
2	B	1857	0	1805	42	0
3	A	1	0	0	0	0
4	A	87	0	0	3	0
4	B	116	0	0	8	0
All	All	3692	0	3416	64	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 9.

All (64) 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:5:HIS:HD2	2:B:60:GLU:HG2	1.05	1.10
2:B:25:ILE:HD11	2:B:28:THR:HG22	1.35	1.07
2:B:5:HIS:CD2	2:B:60:GLU:HG2	1.94	1.01
2:B:210:LYS:HE3	2:B:210:LYS:HA	1.46	0.94
1:A:20:ARG:HD2	4:B:287:HOH:O	1.68	0.93
2:B:2:ASN:HD21	2:B:166:ARG:HH12	1.07	0.93
2:B:5:HIS:HD2	2:B:60:GLU:CG	1.88	0.84
2:B:2:ASN:ND2	2:B:166:ARG:HH12	1.82	0.77
1:A:14:PHE:HB3	1:A:17:HIS:CD2	2.20	0.76
2:B:5:HIS:ND1	2:B:6:ASP:N	2.33	0.76
2:B:159:THR:HG23	2:B:183:ASP:OD1	1.88	0.73
1:A:53:HIS:CD2	1:A:58:LEU:HD22	2.24	0.73
2:B:2:ASN:HD21	2:B:166:ARG:NH1	1.85	0.72
1:A:16:HIS:H	1:A:16:HIS:CD2	2.08	0.70
2:B:54:GLU:OE1	4:B:341:HOH:O	2.09	0.69
1:A:159:PRO:HD2	1:A:162:VAL:HG13	1.77	0.66
2:B:5:HIS:CD2	2:B:60:GLU:CG	2.71	0.65
2:B:60:GLU:OE1	2:B:158:HIS:HD2	1.81	0.64
2:B:5:HIS:C	2:B:5:HIS:ND1	2.50	0.63
2:B:159:THR:HB	2:B:161:PHE:H	1.64	0.62
1:A:41:HIS:HE1	4:B:279:HOH:O	1.82	0.62
2:B:160:ARG:O	2:B:162:PRO:HD3	1.99	0.61
2:B:15:LYS:HG2	2:B:17:MET:CE	2.31	0.61
2:B:88:GLY:HA2	4:B:292:HOH:O	2.00	0.61
2:B:210:LYS:CE	2:B:210:LYS:HA	2.28	0.59
1:A:89:ARG:HG3	1:A:94:TYR:CD1	2.38	0.59
2:B:25:ILE:HD11	2:B:28:THR:CG2	2.24	0.58
1:A:36:LEU:HD13	1:A:42:LEU:HD22	1.84	0.57
2:B:171:VAL:HG22	4:B:282:HOH:O	2.02	0.57
2:B:4:ILE:N	2:B:4:ILE:HD12	2.20	0.57
2:B:93:LYS:NZ	2:B:93:LYS:HB2	2.20	0.56
1:A:16:HIS:N	1:A:16:HIS:CD2	2.73	0.55
2:B:22:GLU:HG2	4:B:255:HOH:O	2.05	0.55
1:A:165:ARG:HD3	4:A:309:HOH:O	2.08	0.54
2:B:159:THR:CG2	2:B:183:ASP:OD1	2.56	0.53
1:A:53:HIS:CD2	1:A:58:LEU:CD2	2.91	0.53
2:B:5:HIS:CE1	2:B:6:ASP:HB2	2.44	0.53
1:A:121:CSO:HB2	1:A:174:ARG:CZ	2.39	0.53
1:A:16:HIS:HD2	1:A:16:HIS:H	1.53	0.52
2:B:158:HIS:HE1	4:B:257:HOH:O	1.94	0.51
4:A:356:HOH:O	2:B:75:HIS:HD2	1.94	0.51
1:A:159:PRO:HD2	1:A:162:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LYS:NZ	2:B:128:ASP:OD2	2.43	0.50
2:B:67:TYR:O	2:B:75:HIS:HE1	1.98	0.47
1:A:172:GLU:HG3	2:B:132:PRO:HG3	1.97	0.47
2:B:183:ASP:OD2	2:B:183:ASP:N	2.48	0.47
4:A:310:HOH:O	2:B:214:SER:HB2	2.14	0.46
1:A:115:VAL:HG22	1:A:116:CYS:N	2.31	0.46
2:B:210:LYS:CE	2:B:211:GLN:H	2.28	0.45
2:B:210:LYS:HE2	2:B:211:GLN:H	1.81	0.45
2:B:4:ILE:HD12	2:B:4:ILE:H	1.82	0.44
2:B:136:ILE:HD11	2:B:195:TYR:CE1	2.54	0.43
1:A:59:GLY:HA3	1:A:61:MET:SD	2.59	0.43
1:A:177:VAL:O	1:A:179:PRO:HD3	2.20	0.42
2:B:103:LEU:HD12	2:B:103:LEU:HA	1.96	0.42
1:A:53:HIS:HA	1:A:57:GLU:HB2	2.02	0.42
1:A:120:SER:HB2	1:A:135:LYS:HG2	2.02	0.41
1:A:165:ARG:HB3	2:B:216:TYR:CE1	2.56	0.41
2:B:148:ILE:HD12	2:B:148:ILE:C	2.40	0.41
2:B:91:ASP:N	4:B:313:HOH:O	2.54	0.41
2:B:150:THR:HB	2:B:161:PHE:CZ	2.56	0.41
1:A:42:LEU:HA	1:A:42:LEU:HD12	1.98	0.41
1:A:185:THR:O	1:A:188:MET:HG2	2.21	0.41
1:A:201:SER:HA	1:A:206:ALA:O	2.21	0.41

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	198/216 (92%)	191 (96%)	6 (3%)	1 (0%)	34	55
2	B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
All	All	423/445 (95%)	407 (96%)	15 (4%)	1 (0%)	52	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	SER

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	177/190 (93%)	165 (93%)	12 (7%)	20	35
2	B	194/196 (99%)	165 (85%)	29 (15%)	4	6
All	All	371/386 (96%)	330 (89%)	41 (11%)	8	13

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	20	ARG
1	A	28	ARG
1	A	32	LEU
1	A	35	LEU
1	A	42	LEU
1	A	52	LYS
1	A	58	LEU
1	A	61	MET
1	A	126	LEU
1	A	165	ARG
1	A	186	GLU
2	B	4	ILE
2	B	5	HIS
2	B	19	VAL
2	B	34	LEU
2	B	36	PHE
2	B	47	LEU
2	B	64	PRO
2	B	65	VAL
2	B	84	LEU
2	B	92	GLU

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Mol	Chain	Res	Type
2	B	93	LYS
2	B	95	LEU
2	B	97	GLU
2	B	103	LEU
2	B	104	LYS
2	B	107	ASP
2	B	109	LYS
2	B	112	ARG
2	B	118	LEU
2	B	121	LEU
2	B	139	SER
2	B	143	LYS
2	B	149	LYS
2	B	159	THR
2	B	166	ARG
2	B	183	ASP
2	B	204	GLU
2	B	210	LYS
2	B	214	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	17	HIS
1	A	41	HIS
1	A	62	ASN
2	B	2	ASN
2	B	29	HIS
2	B	75	HIS
2	B	152	ASN
2	B	158	HIS
2	B	192	ASN
2	B	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSD	A	119	1,3	3,7,8	1.08	0	3,8,10	4.73	2 (66%)
1	CSO	A	121	1,3	3,6,7	1.81	1 (33%)	1,6,8	0.51	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
1	CSD	A	119	1,3	-	0/2/6/8	0/0/0/0
1	CSO	A	121	1,3	-	0/1/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CSO	O-C	3.04	1.33	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	CSD	O-C-CA	-2.26	119.59	125.49
1	A	119	CSD	OD1-SG-CB	7.88	118.54	105.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	121	CSO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

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	200/216 (92%)	-0.13	1 (0%) 91 93	17, 27, 42, 49	0
2	B	227/229 (99%)	-0.13	9 (3%) 42 47	15, 25, 46, 62	0
All	All	427/445 (95%)	-0.13	10 (2%) 64 68	15, 26, 44, 62	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	22	GLU	3.3
2	B	210	LYS	3.1
1	A	78	GLN	2.7
2	B	109	LYS	2.5
2	B	209	TYR	2.5
2	B	104	LYS	2.4
2	B	107	ASP	2.4
2	B	139	SER	2.3
2	B	120	LYS	2.2
2	B	116	PRO	2.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	CSO	A	121	7/8	0.96	0.10	-	19,20,21,27	0
1	CSD	A	119	8/9	0.98	0.09	-	15,18,19,22	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CO	A	301	1/1	0.99	0.03	-	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.