



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 07:21 AM EST

PDB ID : 3VZS
Title : Crystal structure of PhaB from *Ralstonia eutropha* in complex with Acetoacetyl-CoA and NADP
Authors : Ikeda, K.; Tanaka, Y.; Tanaka, I.; Yao, M.
Deposited on : unknown
Resolution : 2.14 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

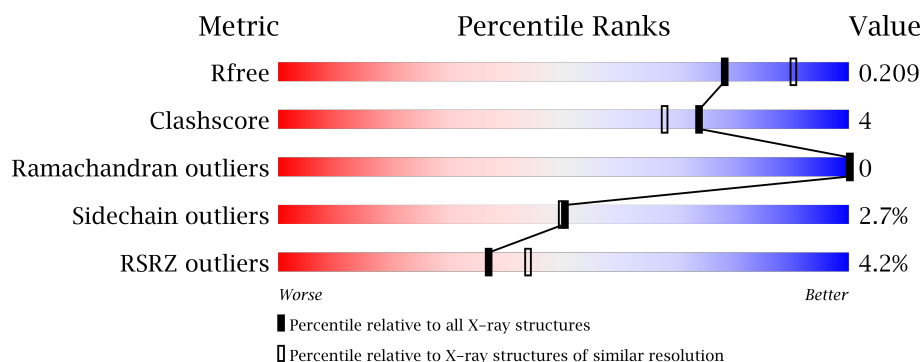
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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	257	<div> <div>0.1%</div> <div>88%</div> <div>6%</div> <div>5%</div> </div>
1	B	257	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>2%</div> </div>
1	C	257	<div> <div>5%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
1	D	257	<div> <div>7%</div> <div>87%</div> <div>9%</div> <div>1%</div> </div>

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.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAP	A	302	-	-	-	X
3	NAP	B	302	-	-	-	X
3	NAP	C	302	-	-	-	X
3	NAP	D	302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8469 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 Acetoacetyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1835	1149	324	353	9			
1	B	249	Total	C	N	O	S	0	0	0
			1872	1170	333	360	9			
1	C	244	Total	C	N	O	S	0	0	0
			1835	1149	324	353	9			
1	D	249	Total	C	N	O	S	0	0	0
			1872	1170	333	360	9			

There are 48 discrepancies between the modelled and reference sequences:

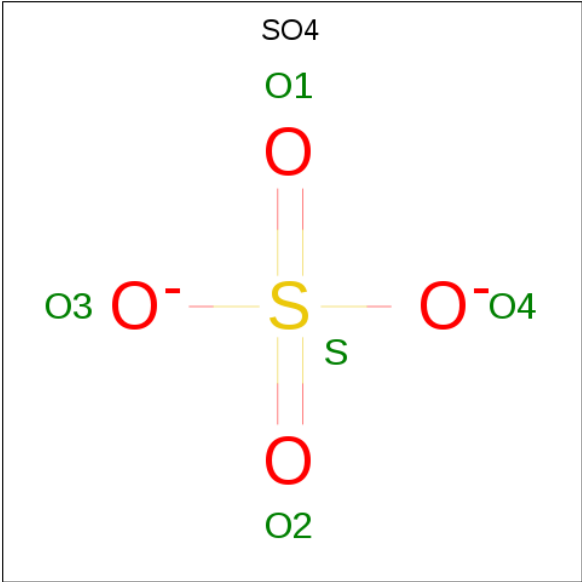
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P14697
A	-9	ARG	-	EXPRESSION TAG	UNP P14697
A	-8	GLY	-	EXPRESSION TAG	UNP P14697
A	-7	SER	-	EXPRESSION TAG	UNP P14697
A	-6	HIS	-	EXPRESSION TAG	UNP P14697
A	-5	HIS	-	EXPRESSION TAG	UNP P14697
A	-4	HIS	-	EXPRESSION TAG	UNP P14697
A	-3	HIS	-	EXPRESSION TAG	UNP P14697
A	-2	HIS	-	EXPRESSION TAG	UNP P14697
A	-1	HIS	-	EXPRESSION TAG	UNP P14697
A	0	GLY	-	EXPRESSION TAG	UNP P14697
A	1	SER	-	EXPRESSION TAG	UNP P14697
B	-10	MET	-	EXPRESSION TAG	UNP P14697
B	-9	ARG	-	EXPRESSION TAG	UNP P14697
B	-8	GLY	-	EXPRESSION TAG	UNP P14697
B	-7	SER	-	EXPRESSION TAG	UNP P14697
B	-6	HIS	-	EXPRESSION TAG	UNP P14697
B	-5	HIS	-	EXPRESSION TAG	UNP P14697
B	-4	HIS	-	EXPRESSION TAG	UNP P14697
B	-3	HIS	-	EXPRESSION TAG	UNP P14697
B	-2	HIS	-	EXPRESSION TAG	UNP P14697

Continued on next page...

Continued from previous page...

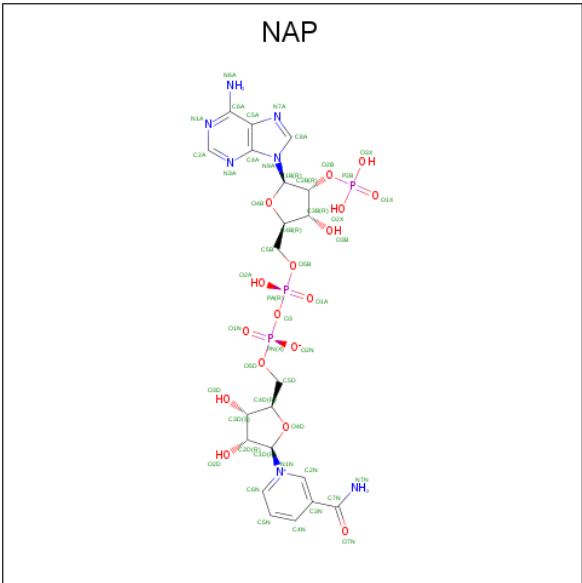
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	HIS	-	EXPRESSION TAG	UNP P14697
B	0	GLY	-	EXPRESSION TAG	UNP P14697
B	1	SER	-	EXPRESSION TAG	UNP P14697
C	-10	MET	-	EXPRESSION TAG	UNP P14697
C	-9	ARG	-	EXPRESSION TAG	UNP P14697
C	-8	GLY	-	EXPRESSION TAG	UNP P14697
C	-7	SER	-	EXPRESSION TAG	UNP P14697
C	-6	HIS	-	EXPRESSION TAG	UNP P14697
C	-5	HIS	-	EXPRESSION TAG	UNP P14697
C	-4	HIS	-	EXPRESSION TAG	UNP P14697
C	-3	HIS	-	EXPRESSION TAG	UNP P14697
C	-2	HIS	-	EXPRESSION TAG	UNP P14697
C	-1	HIS	-	EXPRESSION TAG	UNP P14697
C	0	GLY	-	EXPRESSION TAG	UNP P14697
C	1	SER	-	EXPRESSION TAG	UNP P14697
D	-10	MET	-	EXPRESSION TAG	UNP P14697
D	-9	ARG	-	EXPRESSION TAG	UNP P14697
D	-8	GLY	-	EXPRESSION TAG	UNP P14697
D	-7	SER	-	EXPRESSION TAG	UNP P14697
D	-6	HIS	-	EXPRESSION TAG	UNP P14697
D	-5	HIS	-	EXPRESSION TAG	UNP P14697
D	-4	HIS	-	EXPRESSION TAG	UNP P14697
D	-3	HIS	-	EXPRESSION TAG	UNP P14697
D	-2	HIS	-	EXPRESSION TAG	UNP P14697
D	-1	HIS	-	EXPRESSION TAG	UNP P14697
D	0	GLY	-	EXPRESSION TAG	UNP P14697
D	1	SER	-	EXPRESSION TAG	UNP P14697

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



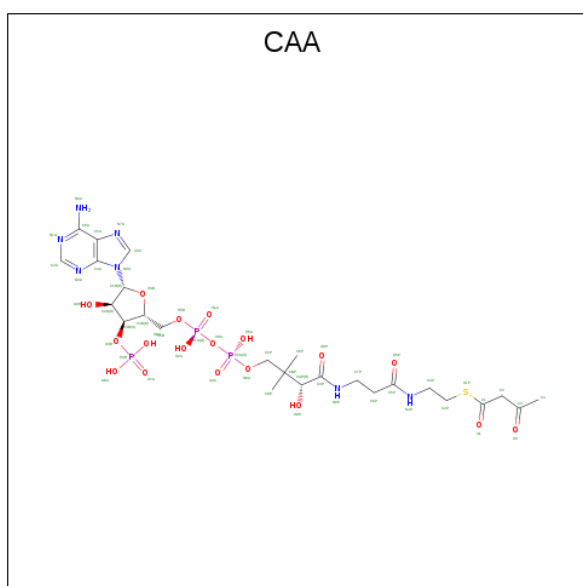
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total	O	0	0
			182	182		
5	B	162	Total	O	0	0
			162	162		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	145	Total	O	0	0
			145	145		
5	D	138	Total	O	0	0
			138	138		

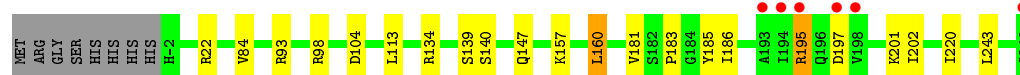
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

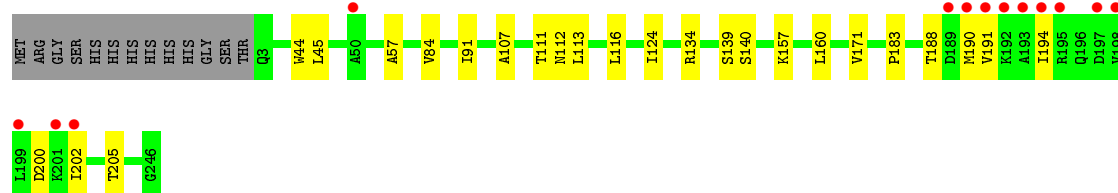
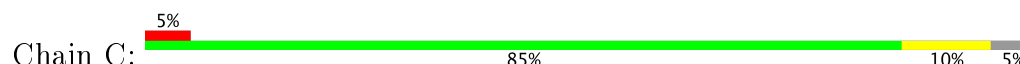
- Molecule 1: Acetoacetyl-CoA reductase



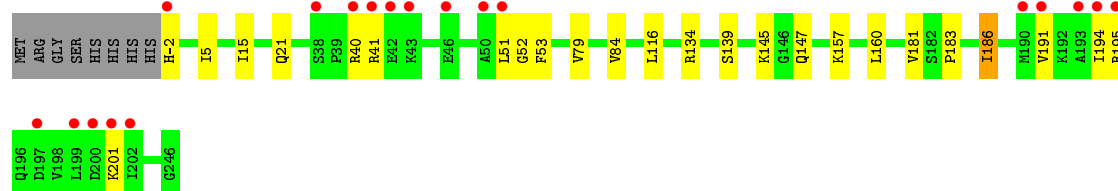
- Molecule 1: Acetoacetyl-CoA reductase



- Molecule 1: Acetoacetyl-CoA reductase



- Molecule 1: Acetoacetyl-CoA reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	67.40 Å 123.44 Å 260.25 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.12 – 2.14 35.12 – 2.14	Depositor EDS
% Data completeness (in resolution range)	96.6 (35.12-2.14) 96.6 (35.12-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.05 (at 2.14 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.165 , 0.209 0.166 , 0.209	Depositor DCC
R_{free} test set	2948 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.044 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8469	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, CAA, 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	A	0.21	0/1864	0.40	0/2520
1	B	0.21	0/1903	0.42	1/2573 (0.0%)
1	C	0.21	0/1864	0.39	0/2520
1	D	0.21	0/1903	0.41	0/2573
All	All	0.21	0/7534	0.40	1/10186 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1835	0	1829	11	0
1	B	1872	0	1861	12	0
1	C	1835	0	1829	17	0
1	D	1872	0	1861	15	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	48	0	24	4	0
3	B	48	0	24	1	0
3	C	48	0	24	2	0
3	D	48	0	24	5	0
4	A	54	0	36	1	0
4	B	54	0	36	2	0
4	C	54	0	36	0	0
4	D	54	0	36	1	0
5	A	182	0	0	0	0
5	B	162	0	0	1	0
5	C	145	0	0	0	0
5	D	138	0	0	0	0
All	All	8469	0	7620	59	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 4.

All (59) 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)
3:D:302:NAP:H71N	4:D:303:CAA:H4'1	1.45	0.81
4:A:303:CAA:H8A	4:A:303:CAA:H51A	1.71	0.71
1:A:195:ARG:H	1:A:195:ARG:HE	1.39	0.71
1:D:51:LEU:N	1:D:52:GLY:HA2	2.14	0.62
1:B:195:ARG:HD2	1:B:195:ARG:H	1.65	0.62
1:A:84:VAL:HG22	1:A:134:ARG:HB2	1.82	0.61
1:D:139:SER:HB2	1:D:160:LEU:HD22	1.83	0.58
1:B:139:SER:HB2	1:B:160:LEU:HD11	1.86	0.58
4:B:303:CAA:O7A	4:B:303:CAA:H4B	2.04	0.57
1:C:44:TRP:HE3	1:C:45:LEU:HD12	1.69	0.57
1:A:195:ARG:H	1:A:195:ARG:NE	2.02	0.56
1:D:186:ILE:H	3:D:302:NAP:H4N	1.70	0.56
1:B:147:GLN:HE21	4:B:303:CAA:H62	1.71	0.56
1:A:139:SER:HB2	1:A:160:LEU:HD22	1.88	0.56
1:C:84:VAL:HG22	1:C:134:ARG:HB2	1.88	0.55
1:B:22:ARG:NH2	5:B:550:HOH:O	2.32	0.54
1:D:183:PRO:HB2	3:D:302:NAP:N7N	2.23	0.54
1:D:191:VAL:HA	1:D:194:ILE:HG13	1.90	0.53
1:A:183:PRO:HB2	3:A:302:NAP:N7N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:SER:HA	1:B:157:LYS:HD2	1.91	0.52
1:C:139:SER:HB2	1:C:160:LEU:HD22	1.92	0.52
1:D:15:ILE:HG13	1:D:186:ILE:HD11	1.92	0.51
1:C:188:THR:OG1	3:C:302:NAP:H6N	2.11	0.51
1:C:45:LEU:HD11	1:C:57:ALA:HB2	1.91	0.51
1:C:139:SER:HA	1:C:157:LYS:HD2	1.94	0.50
1:D:15:ILE:H	1:D:15:ILE:HD12	1.75	0.50
1:C:191:VAL:HA	1:C:194:ILE:HG13	1.95	0.48
1:D:51:LEU:H	1:D:52:GLY:HA2	1.79	0.48
1:D:139:SER:HA	1:D:157:LYS:HD2	1.95	0.47
1:B:84:VAL:HG22	1:B:134:ARG:HB2	1.95	0.47
1:A:139:SER:HA	1:A:157:LYS:HD2	1.97	0.47
1:A:191:VAL:HA	1:A:194:ILE:HG13	1.98	0.46
1:B:185:TYR:CE2	1:B:202:ILE:HD13	2.50	0.46
1:B:201:LYS:HB2	1:B:201:LYS:HE3	1.83	0.45
1:D:186:ILE:H	3:D:302:NAP:C4N	2.28	0.45
3:A:302:NAP:H2N	3:A:302:NAP:H2D	1.74	0.45
1:B:139:SER:OG	1:B:140:SER:N	2.50	0.45
1:D:5:ILE:HD13	1:D:79:VAL:HG12	1.98	0.45
1:A:202:ILE:O	1:A:205:THR:OG1	2.28	0.44
1:D:183:PRO:HB2	3:D:302:NAP:H72N	1.81	0.44
1:B:186:ILE:HG12	3:B:302:NAP:H4N	1.98	0.44
1:C:202:ILE:O	1:C:205:THR:OG1	2.33	0.44
1:C:113:LEU:HD12	1:C:116:LEU:HD12	2.00	0.43
1:D:181:VAL:O	1:D:183:PRO:HD3	2.18	0.43
1:C:112:ASN:HD22	1:C:157:LYS:HE2	1.82	0.43
1:C:111:THR:HG23	1:C:112:ASN:OD1	2.19	0.42
1:A:38:SER:HA	1:A:39:PRO:HD3	1.83	0.42
1:B:181:VAL:O	1:B:183:PRO:HD3	2.19	0.42
1:B:93:ARG:HG2	1:B:104:ASP:HA	2.00	0.42
1:C:113:LEU:HA	1:C:113:LEU:HD12	1.89	0.41
1:A:188:THR:OG1	3:A:302:NAP:H6N	2.21	0.41
1:C:183:PRO:HB2	3:C:302:NAP:O7N	2.20	0.41
1:D:21:GLN:HB2	1:D:53:PHE:CZ	2.55	0.41
1:D:201:LYS:HE3	1:D:201:LYS:HB2	1.79	0.41
1:A:40:ARG:NH2	3:A:302:NAP:O2X	2.41	0.41
1:C:107:ALA:O	1:C:111:THR:HG22	2.21	0.40
1:C:91:ILE:HG12	1:C:111:THR:HG21	2.03	0.40
1:C:139:SER:OG	1:C:140:SER:N	2.54	0.40
1:C:124:ILE:HD11	1:C:171:VAL:HG11	2.03	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	242/257 (94%)	236 (98%)	6 (2%)	0	100	100
1	B	247/257 (96%)	242 (98%)	5 (2%)	0	100	100
1	C	242/257 (94%)	239 (99%)	3 (1%)	0	100	100
1	D	247/257 (96%)	239 (97%)	8 (3%)	0	100	100
All	All	978/1028 (95%)	956 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	193/204 (95%)	190 (98%)	3 (2%)	68	71
1	B	197/204 (97%)	191 (97%)	6 (3%)	46	44
1	C	193/204 (95%)	191 (99%)	2 (1%)	80	83
1	D	197/204 (97%)	187 (95%)	10 (5%)	28	22
All	All	780/816 (96%)	759 (97%)	21 (3%)	50	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	69	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	ARG
1	B	98	ARG
1	B	113	LEU
1	B	195	ARG
1	B	197	ASP
1	B	220	ILE
1	B	243	LEU
1	C	190	MET
1	C	200	ASP
1	D	-2	HIS
1	D	40	ARG
1	D	41	ARG
1	D	84	VAL
1	D	116	LEU
1	D	134	ARG
1	D	145	LYS
1	D	147	GLN
1	D	186	ILE
1	D	195	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	147	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 carbohydrates in this entry.

5.6 Ligand geometry

12 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
2	SO4	A	301	-	4,4,4	0.13	0	6,6,6	0.06	0
3	NAP	A	302	-	44,52,52	2.16	13 (29%)	51,80,80	1.73	7 (13%)
4	CAA	A	303	-	49,56,56	1.71	8 (16%)	57,83,83	1.84	12 (21%)
2	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.05	0
3	NAP	B	302	-	44,52,52	2.15	13 (29%)	51,80,80	1.76	8 (15%)
4	CAA	B	303	-	49,56,56	1.74	8 (16%)	57,83,83	1.95	11 (19%)
2	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.06	0
3	NAP	C	302	-	44,52,52	2.16	13 (29%)	51,80,80	1.76	8 (15%)
4	CAA	C	303	-	49,56,56	1.73	8 (16%)	57,83,83	1.89	11 (19%)
2	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.05	0
3	NAP	D	302	-	44,52,52	2.16	13 (29%)	51,80,80	1.86	7 (13%)
4	CAA	D	303	-	49,56,56	1.72	8 (16%)	57,83,83	1.88	10 (17%)

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
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
3	NAP	A	302	-	-	0/27/67/67	0/5/5/5
4	CAA	A	303	-	-	2/50/71/71	0/3/3/3
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
3	NAP	B	302	-	-	0/27/67/67	0/5/5/5
4	CAA	B	303	-	-	2/50/71/71	0/3/3/3
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
3	NAP	C	302	-	-	0/27/67/67	0/5/5/5
4	CAA	C	303	-	-	2/50/71/71	0/3/3/3
2	SO4	D	301	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	D	302	-	-	0/27/67/67	0/5/5/5
4	CAA	D	303	-	-	2/50/71/71	0/3/3/3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	CAA	C2B-C3B	-5.50	1.40	1.53
4	B	303	CAA	C2B-C3B	-5.37	1.41	1.53
4	A	303	CAA	C2B-C3B	-5.29	1.41	1.53
4	D	303	CAA	C2B-C3B	-5.24	1.41	1.53
4	C	303	CAA	C2B-C1B	-3.46	1.48	1.53
3	D	302	NAP	C2D-C3D	-3.37	1.44	1.53
3	B	302	NAP	C2D-C3D	-3.29	1.44	1.53
3	A	302	NAP	C2D-C3D	-3.26	1.44	1.53
3	C	302	NAP	C2D-C3D	-3.24	1.44	1.53
4	D	303	CAA	C2B-C1B	-3.20	1.48	1.53
3	C	302	NAP	C3B-C2B	-3.16	1.46	1.53
3	B	302	NAP	C3B-C2B	-3.15	1.46	1.53
3	D	302	NAP	C3B-C2B	-3.14	1.46	1.53
3	B	302	NAP	O2D-C2D	-3.14	1.35	1.43
3	A	302	NAP	C3B-C2B	-3.13	1.46	1.53
3	C	302	NAP	O2D-C2D	-3.09	1.35	1.43
3	A	302	NAP	O2D-C2D	-3.08	1.35	1.43
3	D	302	NAP	O2D-C2D	-3.07	1.35	1.43
4	A	303	CAA	C2B-C1B	-3.04	1.48	1.53
4	B	303	CAA	C2B-C1B	-2.84	1.49	1.53
4	B	303	CAA	O4B-C4B	-2.83	1.38	1.45
4	D	303	CAA	O4B-C4B	-2.74	1.38	1.45
4	A	303	CAA	O4B-C4B	-2.70	1.38	1.45
4	C	303	CAA	O4B-C4B	-2.58	1.39	1.45
4	B	303	CAA	C3B-C4B	-2.51	1.45	1.52
3	C	302	NAP	O3B-C3B	-2.47	1.37	1.43
3	B	302	NAP	O3B-C3B	-2.45	1.37	1.43
3	D	302	NAP	O3D-C3D	-2.43	1.37	1.43
3	A	302	NAP	O3B-C3B	-2.43	1.37	1.43
3	D	302	NAP	O3B-C3B	-2.43	1.37	1.43
3	C	302	NAP	O3D-C3D	-2.42	1.37	1.43
3	A	302	NAP	O3D-C3D	-2.41	1.37	1.43
4	A	303	CAA	C3B-C4B	-2.37	1.46	1.52
3	B	302	NAP	O3D-C3D	-2.37	1.37	1.43
4	C	303	CAA	C3B-C4B	-2.30	1.46	1.52
4	D	303	CAA	C3B-C4B	-2.29	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	NAP	O4B-C4B	-2.27	1.39	1.45
3	D	302	NAP	O4D-C4D	-2.27	1.39	1.45
3	A	302	NAP	O4B-C4B	-2.26	1.39	1.45
3	C	302	NAP	O4B-C4B	-2.24	1.39	1.45
3	B	302	NAP	O4B-C4B	-2.21	1.40	1.45
3	C	302	NAP	O4D-C4D	-2.20	1.40	1.45
3	B	302	NAP	O4D-C4D	-2.18	1.40	1.45
3	A	302	NAP	O4D-C4D	-2.16	1.40	1.45
3	D	302	NAP	C3B-C4B	-2.11	1.47	1.53
3	B	302	NAP	C3B-C4B	-2.10	1.47	1.53
3	C	302	NAP	C3B-C4B	-2.10	1.47	1.53
3	A	302	NAP	C3B-C4B	-2.06	1.47	1.53
4	A	303	CAA	C6A-N6A	2.11	1.42	1.34
4	D	303	CAA	C6A-N6A	2.11	1.42	1.34
4	C	303	CAA	C6A-N6A	2.12	1.42	1.34
3	C	302	NAP	C2A-N3A	2.17	1.35	1.32
4	B	303	CAA	C6A-N6A	2.18	1.43	1.34
3	B	302	NAP	C2A-N3A	2.21	1.35	1.32
3	A	302	NAP	C2A-N3A	2.21	1.35	1.32
3	D	302	NAP	C2A-N3A	2.24	1.35	1.32
4	C	303	CAA	C2A-N3A	2.38	1.36	1.32
4	A	303	CAA	C2A-N3A	2.39	1.36	1.32
4	D	303	CAA	C2A-N3A	2.43	1.36	1.32
4	B	303	CAA	C2A-N3A	2.46	1.36	1.32
3	A	302	NAP	C6A-N6A	3.37	1.47	1.34
3	D	302	NAP	C6A-N6A	3.38	1.47	1.34
3	C	302	NAP	C6A-N6A	3.39	1.48	1.34
3	B	302	NAP	C6A-N6A	3.40	1.48	1.34
3	A	302	NAP	O4B-C1B	3.68	1.46	1.41
3	D	302	NAP	O4B-C1B	3.79	1.46	1.41
3	B	302	NAP	O4B-C1B	3.84	1.46	1.41
3	C	302	NAP	O4B-C1B	3.89	1.46	1.41
4	A	303	CAA	C9P-N8P	4.95	1.43	1.33
4	C	303	CAA	C9P-N8P	5.04	1.43	1.33
4	B	303	CAA	C9P-N8P	5.05	1.43	1.33
4	D	303	CAA	C9P-N8P	5.08	1.44	1.33
3	A	302	NAP	C7N-N7N	5.50	1.43	1.33
3	D	302	NAP	C7N-N7N	5.59	1.43	1.33
3	C	302	NAP	C7N-N7N	5.62	1.44	1.33
3	B	302	NAP	C7N-N7N	5.65	1.44	1.33
4	C	303	CAA	C5P-N4P	5.93	1.47	1.33
4	A	303	CAA	C5P-N4P	5.95	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	303	CAA	C5P-N4P	5.98	1.47	1.33
4	B	303	CAA	C5P-N4P	6.04	1.47	1.33
3	B	302	NAP	O4D-C1D	8.43	1.52	1.41
3	D	302	NAP	O4D-C1D	8.47	1.53	1.41
3	C	302	NAP	O4D-C1D	8.52	1.53	1.41
3	A	302	NAP	O4D-C1D	8.70	1.53	1.41

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	NAP	N3A-C2A-N1A	-8.49	121.47	128.86
3	A	302	NAP	N3A-C2A-N1A	-8.48	121.47	128.86
3	B	302	NAP	N3A-C2A-N1A	-8.38	121.56	128.86
3	C	302	NAP	N3A-C2A-N1A	-8.37	121.57	128.86
4	D	303	CAA	N3A-C2A-N1A	-7.33	122.47	128.86
4	C	303	CAA	N3A-C2A-N1A	-7.30	122.50	128.86
4	A	303	CAA	N3A-C2A-N1A	-7.14	122.64	128.86
4	B	303	CAA	N3A-C2A-N1A	-6.89	122.86	128.86
3	D	302	NAP	C4D-O4D-C1D	-6.36	103.00	109.77
4	B	303	CAA	O1-C1-S1P	-5.75	116.82	122.84
4	B	303	CAA	O1-C1-C2	-4.87	115.74	123.08
3	C	302	NAP	C4D-O4D-C1D	-4.84	104.62	109.77
3	B	302	NAP	C4D-O4D-C1D	-4.81	104.65	109.77
4	C	303	CAA	O1-C1-S1P	-4.68	117.94	122.84
3	A	302	NAP	C4D-O4D-C1D	-4.42	105.06	109.77
4	A	303	CAA	O1-C1-S1P	-4.06	118.58	122.84
4	B	303	CAA	C4A-C5A-N7A	-3.80	105.74	109.41
4	D	303	CAA	C4A-C5A-N7A	-3.41	106.12	109.41
4	C	303	CAA	C4A-C5A-N7A	-3.33	106.19	109.41
4	A	303	CAA	C4A-C5A-N7A	-3.31	106.21	109.41
4	C	303	CAA	O1-C1-C2	-3.12	118.39	123.08
4	A	303	CAA	O1-C1-C2	-3.05	118.49	123.08
3	C	302	NAP	O7N-C7N-N7N	-2.90	118.46	122.58
3	A	302	NAP	O7N-C7N-N7N	-2.78	118.63	122.58
4	D	303	CAA	O1-C1-S1P	-2.72	119.99	122.84
3	D	302	NAP	C5N-C4N-C3N	-2.55	117.35	120.35
3	B	302	NAP	C5N-C4N-C3N	-2.38	117.56	120.35
3	C	302	NAP	C5N-C4N-C3N	-2.29	117.65	120.35
3	A	302	NAP	C5N-C4N-C3N	-2.27	117.68	120.35
3	B	302	NAP	O7N-C7N-N7N	-2.25	119.39	122.58
3	D	302	NAP	O7N-C7N-N7N	-2.13	119.55	122.58
3	A	302	NAP	C4A-C5A-N7A	-2.11	107.37	109.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	NAP	C4A-C5A-N7A	-2.10	107.38	109.41
3	C	302	NAP	C4A-C5A-N7A	-2.10	107.38	109.41
4	A	303	CAA	C4B-O4B-C1B	-2.07	107.57	109.77
3	D	302	NAP	C4A-C5A-N7A	-2.06	107.42	109.41
4	C	303	CAA	C2P-S1P-C1	2.10	108.86	101.90
3	B	302	NAP	O5D-C5D-C4D	2.13	116.55	109.00
4	B	303	CAA	C6P-C7P-N8P	2.15	116.32	111.87
3	A	302	NAP	O5B-C5B-C4B	2.17	116.70	109.00
4	B	303	CAA	CDP-CBP-CAP	2.18	112.59	108.82
4	A	303	CAA	C2P-S1P-C1	2.21	109.20	101.90
4	C	303	CAA	O5B-C5B-C4B	2.23	116.92	109.00
4	D	303	CAA	C2P-C3P-N4P	2.29	117.54	112.49
4	A	303	CAA	C7P-C6P-C5P	2.32	115.95	112.22
3	B	302	NAP	O5B-C5B-C4B	2.44	117.64	109.00
4	D	303	CAA	C3B-C2B-C1B	2.45	105.45	99.95
4	A	303	CAA	C2P-C3P-N4P	2.46	117.92	112.49
4	B	303	CAA	O5B-C5B-C4B	2.46	117.74	109.00
4	C	303	CAA	C2P-C3P-N4P	2.49	117.99	112.49
4	A	303	CAA	O5B-C5B-C4B	2.58	118.16	109.00
3	C	302	NAP	O5D-C5D-C4D	2.63	118.31	109.00
4	A	303	CAA	C6P-C7P-N8P	2.63	117.31	111.87
3	D	302	NAP	O5B-C5B-C4B	2.66	118.45	109.00
4	C	303	CAA	C7P-C6P-C5P	2.68	116.53	112.22
3	C	302	NAP	O5B-C5B-C4B	2.76	118.78	109.00
4	D	303	CAA	C7P-C6P-C5P	2.76	116.66	112.22
4	B	303	CAA	C7P-C6P-C5P	2.78	116.70	112.22
4	D	303	CAA	C6P-C7P-N8P	2.80	117.66	111.87
4	C	303	CAA	C6P-C7P-N8P	2.82	117.71	111.87
4	D	303	CAA	O5B-C5B-C4B	3.00	119.64	109.00
4	A	303	CAA	O6A-CCP-CBP	3.01	115.38	110.55
4	B	303	CAA	C2P-C3P-N4P	3.07	119.26	112.49
4	B	303	CAA	O6A-CCP-CBP	3.60	116.34	110.55
3	D	302	NAP	C3N-C7N-N7N	3.71	122.00	117.77
3	C	302	NAP	C3N-C7N-N7N	3.71	122.01	117.77
3	A	302	NAP	C3N-C7N-N7N	3.92	122.25	117.77
3	B	302	NAP	C3N-C7N-N7N	3.96	122.29	117.77
4	C	303	CAA	O6A-CCP-CBP	4.11	117.15	110.55
4	B	303	CAA	C2-C1-S1P	4.79	118.50	113.42
4	D	303	CAA	O6A-CCP-CBP	4.85	118.35	110.55
4	C	303	CAA	C2-C1-S1P	5.01	118.73	113.42
4	A	303	CAA	C2-C1-S1P	5.50	119.25	113.42
4	D	303	CAA	C2-C1-S1P	5.92	119.70	113.42

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	CAA	C2-C1-S1P-C2P
4	D	303	CAA	C2-C1-S1P-C2P
4	D	303	CAA	O1-C1-S1P-C2P
4	C	303	CAA	C2-C1-S1P-C2P
4	A	303	CAA	C2-C1-S1P-C2P
4	C	303	CAA	O1-C1-S1P-C2P
4	B	303	CAA	O1-C1-S1P-C2P
4	A	303	CAA	O1-C1-S1P-C2P

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	NAP	4	0
4	A	303	CAA	1	0
3	B	302	NAP	1	0
4	B	303	CAA	2	0
3	C	302	NAP	2	0
3	D	302	NAP	5	0
4	D	303	CAA	1	0

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	244/257 (94%)	-0.37	3 (1%) 79 83	5, 12, 29, 54	0
1	B	249/257 (96%)	-0.21	6 (2%) 59 65	7, 13, 33, 59	0
1	C	244/257 (94%)	-0.12	13 (5%) 27 33	6, 13, 45, 69	0
1	D	249/257 (96%)	0.12	19 (7%) 15 18	6, 16, 48, 71	0
All	All	986/1028 (95%)	-0.14	41 (4%) 37 44	5, 13, 41, 71	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	ALA	6.2
1	D	199	LEU	6.1
1	C	195	ARG	5.7
1	D	195	ARG	5.3
1	D	193	ALA	5.1
1	C	199	LEU	5.0
1	A	195	ARG	4.8
1	B	195	ARG	4.6
1	D	197	ASP	4.2
1	D	51	LEU	4.0
1	C	191	VAL	3.7
1	D	194	ILE	3.7
1	C	198	VAL	3.6
1	B	197	ASP	3.3
1	D	42	GLU	3.3
1	A	193	ALA	3.2
1	C	194	ILE	3.2
1	D	43	LYS	3.0
1	C	197	ASP	2.9
1	D	201	LYS	2.9
1	D	200	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	46	GLU	2.8
1	D	50	ALA	2.8
1	D	-2	HIS	2.7
1	B	194	ILE	2.6
1	B	246	GLY	2.5
1	D	190	MET	2.5
1	C	192	LYS	2.5
1	B	198	VAL	2.4
1	D	191	VAL	2.4
1	D	40	ARG	2.3
1	C	189	ASP	2.3
1	C	201	LYS	2.2
1	C	190	MET	2.2
1	A	197	ASP	2.2
1	D	38	SER	2.2
1	C	202	ILE	2.1
1	B	193	ALA	2.1
1	C	50	ALA	2.1
1	D	41	ARG	2.1
1	D	202	ILE	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 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(Å ²)	Q<0.9
3	NAP	C	302	48/48	0.79	0.30	3.27	19,47,75,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAP	D	302	48/48	0.80	0.31	3.02	25,54,76,77	0
3	NAP	B	302	48/48	0.91	0.19	2.87	12,26,57,70	0
3	NAP	A	302	48/48	0.93	0.14	2.01	13,22,47,60	0
4	CAA	A	303	54/54	0.77	0.26	1.41	9,34,81,114	0
4	CAA	D	303	54/54	0.77	0.29	1.27	18,45,97,110	0
4	CAA	B	303	54/54	0.84	0.24	1.23	13,38,91,113	0
4	CAA	C	303	54/54	0.77	0.30	1.22	15,56,107,124	0
2	SO4	A	301	5/5	0.98	0.14	1.14	33,35,44,44	0
2	SO4	C	301	5/5	0.92	0.18	0.01	64,69,76,84	0
2	SO4	D	301	5/5	0.97	0.14	-0.60	42,47,49,65	0
2	SO4	B	301	5/5	0.98	0.09	-0.89	33,34,37,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.