Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 05:02 pm GMT

PDB ID	:	6YAB
Title	:	Crystal structure of PnrA from S. pneumoniae in complex with uridine
Authors	:	Batuecas, M.T.; Hermoso, J.A.
Deposited on	:	2020-03-12
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

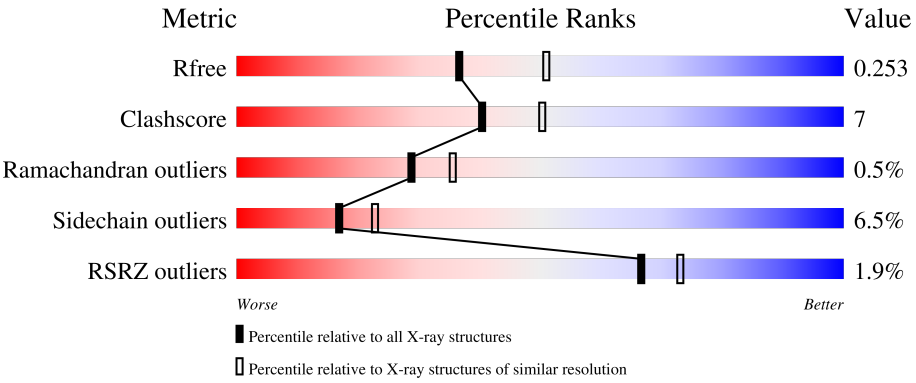
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	BBB	331	83% 14%
1	CCC	331	80% 18%
2	AAA	329	83% 15%
3	DDD	330	5% 86% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NI	DDD	401	-	-	X	-
7	ACT	BBB	404	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10272 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 Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CCC	331	Total	C	N	O	S	0	1	0
			2483	1552	424	506	1			
1	BBB	330	Total	C	N	O	S	0	1	0
			2477	1549	423	504	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	3	SER	-	expression tag	UNP A0A0H2UPF3
CCC	4	SER	-	expression tag	UNP A0A0H2UPF3
CCC	5	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	6	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	7	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	8	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	9	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	10	HIS	-	expression tag	UNP A0A0H2UPF3
CCC	11	MET	-	expression tag	UNP A0A0H2UPF3
CCC	12	SER	-	expression tag	UNP A0A0H2UPF3
CCC	13	GLY	-	expression tag	UNP A0A0H2UPF3
CCC	14	GLU	-	expression tag	UNP A0A0H2UPF3
CCC	15	ASN	-	expression tag	UNP A0A0H2UPF3
CCC	16	LEU	-	expression tag	UNP A0A0H2UPF3
CCC	17	TYR	-	expression tag	UNP A0A0H2UPF3
CCC	18	PHE	-	expression tag	UNP A0A0H2UPF3
CCC	19	GLN	-	expression tag	UNP A0A0H2UPF3
CCC	20	GLY	-	expression tag	UNP A0A0H2UPF3
CCC	21	ALA	-	expression tag	UNP A0A0H2UPF3
CCC	22	SER	-	expression tag	UNP A0A0H2UPF3
BBB	3	SER	-	expression tag	UNP A0A0H2UPF3
BBB	4	SER	-	expression tag	UNP A0A0H2UPF3
BBB	5	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	6	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	7	HIS	-	expression tag	UNP A0A0H2UPF3

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	8	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	9	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	10	HIS	-	expression tag	UNP A0A0H2UPF3
BBB	11	MET	-	expression tag	UNP A0A0H2UPF3
BBB	12	SER	-	expression tag	UNP A0A0H2UPF3
BBB	13	GLY	-	expression tag	UNP A0A0H2UPF3
BBB	14	GLU	-	expression tag	UNP A0A0H2UPF3
BBB	15	ASN	-	expression tag	UNP A0A0H2UPF3
BBB	16	LEU	-	expression tag	UNP A0A0H2UPF3
BBB	17	TYR	-	expression tag	UNP A0A0H2UPF3
BBB	18	PHE	-	expression tag	UNP A0A0H2UPF3
BBB	19	GLN	-	expression tag	UNP A0A0H2UPF3
BBB	20	GLY	-	expression tag	UNP A0A0H2UPF3
BBB	21	ALA	-	expression tag	UNP A0A0H2UPF3
BBB	22	SER	-	expression tag	UNP A0A0H2UPF3

- Molecule 2 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AAA	329	Total	C	N	O	S	0	0	0
			2466	1543	421	501	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	5	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	6	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	7	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	8	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	9	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	10	HIS	-	expression tag	UNP A0A0H2UPF3
AAA	11	MET	-	expression tag	UNP A0A0H2UPF3
AAA	12	SER	-	expression tag	UNP A0A0H2UPF3
AAA	13	GLY	-	expression tag	UNP A0A0H2UPF3
AAA	14	GLU	-	expression tag	UNP A0A0H2UPF3
AAA	15	ASN	-	expression tag	UNP A0A0H2UPF3
AAA	16	LEU	-	expression tag	UNP A0A0H2UPF3
AAA	17	TYR	-	expression tag	UNP A0A0H2UPF3
AAA	18	PHE	-	expression tag	UNP A0A0H2UPF3
AAA	19	GLN	-	expression tag	UNP A0A0H2UPF3
AAA	20	GLY	-	expression tag	UNP A0A0H2UPF3
AAA	21	ALA	-	expression tag	UNP A0A0H2UPF3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	22	SER	-	expression tag	UNP A0A0H2UPF3

- Molecule 3 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	329	Total	C	N	O	S	0	0	0
			2463	1540	420	502	1			

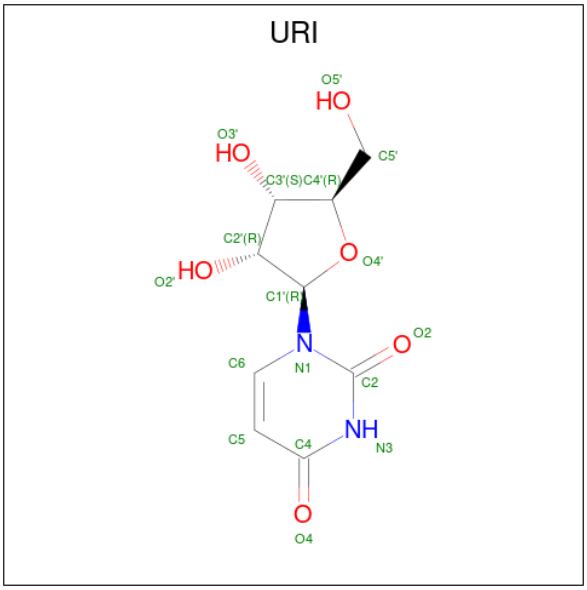
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	3	SER	-	expression tag	UNP A0A0H2UPF3
DDD	4	SER	-	expression tag	UNP A0A0H2UPF3
DDD	5	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	6	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	7	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	8	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	9	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	10	HIS	-	expression tag	UNP A0A0H2UPF3
DDD	11	MET	-	expression tag	UNP A0A0H2UPF3
DDD	12	SER	-	expression tag	UNP A0A0H2UPF3
DDD	13	GLY	-	expression tag	UNP A0A0H2UPF3
DDD	14	GLU	-	expression tag	UNP A0A0H2UPF3
DDD	15	ASN	-	expression tag	UNP A0A0H2UPF3
DDD	16	LEU	-	expression tag	UNP A0A0H2UPF3
DDD	17	TYR	-	expression tag	UNP A0A0H2UPF3
DDD	18	PHE	-	expression tag	UNP A0A0H2UPF3
DDD	19	GLN	-	expression tag	UNP A0A0H2UPF3
DDD	20	GLY	-	expression tag	UNP A0A0H2UPF3
DDD	21	ALA	-	expression tag	UNP A0A0H2UPF3
DDD	22	SER	-	expression tag	UNP A0A0H2UPF3

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

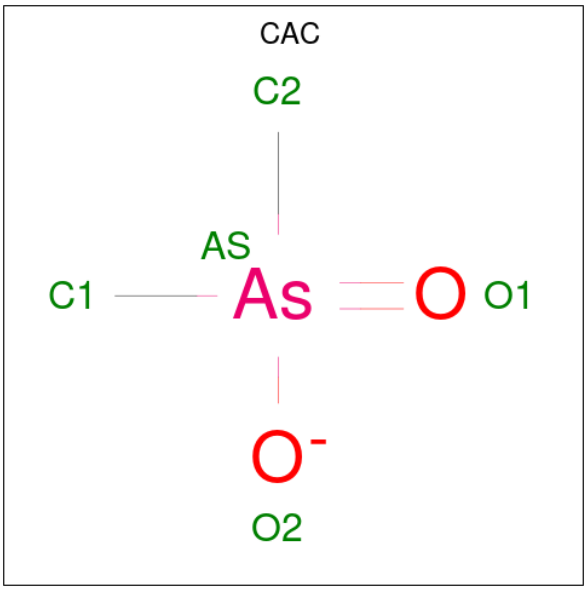
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	CCC	2	Total	Ni	0	0
			2	2		
4	BBB	3	Total	Ni	0	0
			3	3		
4	DDD	4	Total	Ni	0	0
			4	4		

- Molecule 5 is URIDINE (three-letter code: URI) (formula: $C_9H_{12}N_2O_6$).



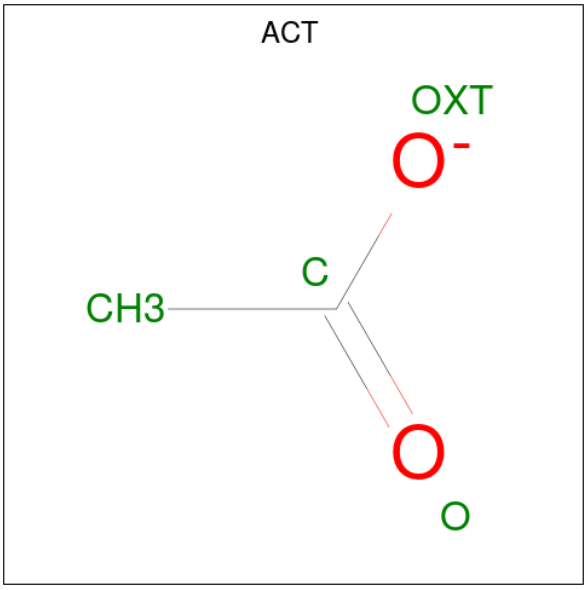
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total C N O 17 9 2 6	0	0
5	AAA	1	Total C N O 17 9 2 6	0	0
5	BBB	1	Total C N O 17 9 2 6	0	0
5	DDD	1	Total C N O 17 9 2 6	0	0

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	CCC	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	BBB	1	Total	C	O		0	0
			4	2	2			
7	BBB	1	Total	C	O		0	0
			4	2	2			

- Molecule 8 is water.

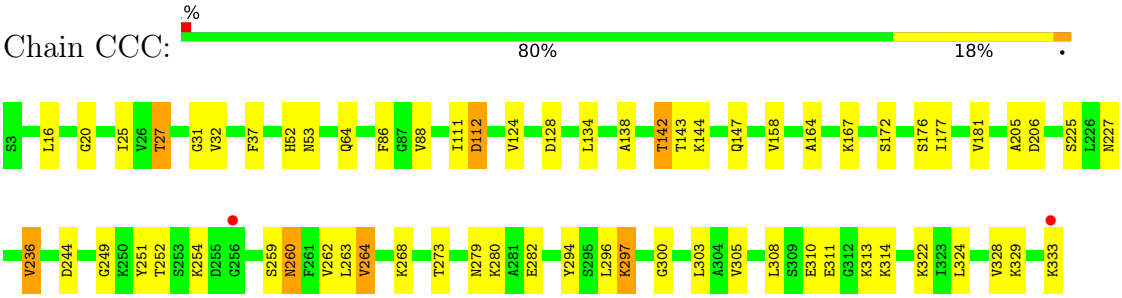
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	CCC	102	Total	O	0	0
			102	102		
8	AAA	84	Total	O	0	0
			84	84		
8	BBB	87	Total	O	0	0
			87	87		
8	DDD	20	Total	O	0	0
			20	20		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

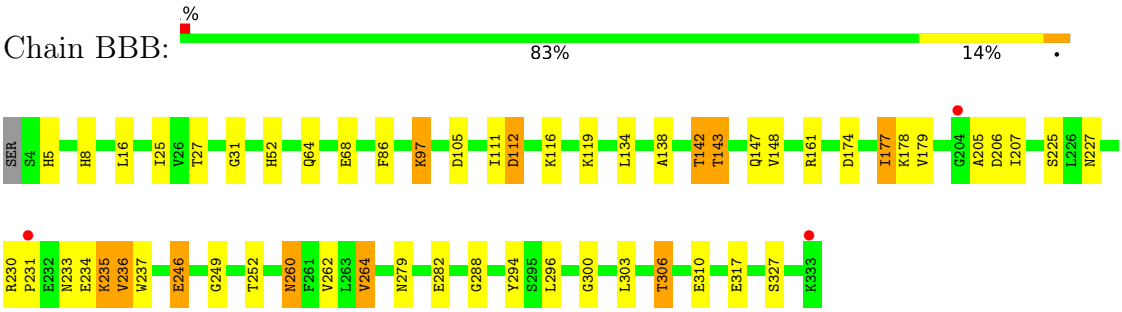
• Molecule 1: Lipoprotein

Chain CCC:



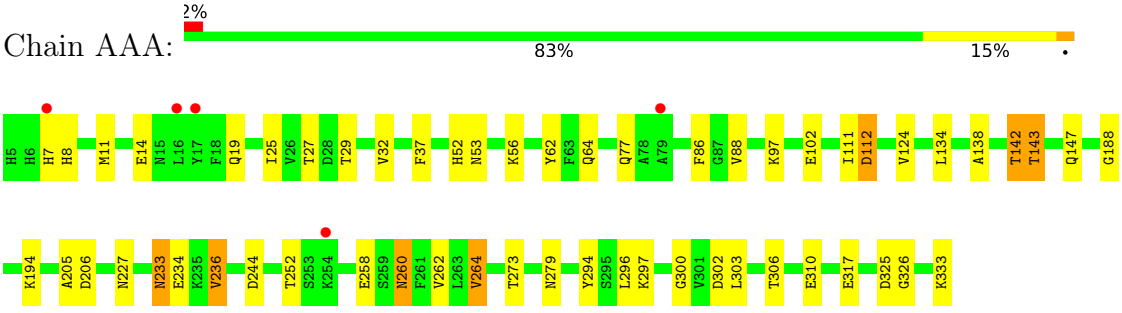
• Molecule 1: Lipoprotein

Chain BBB:



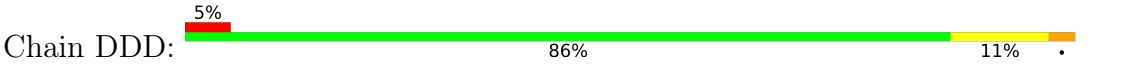
• Molecule 2: Lipoprotein

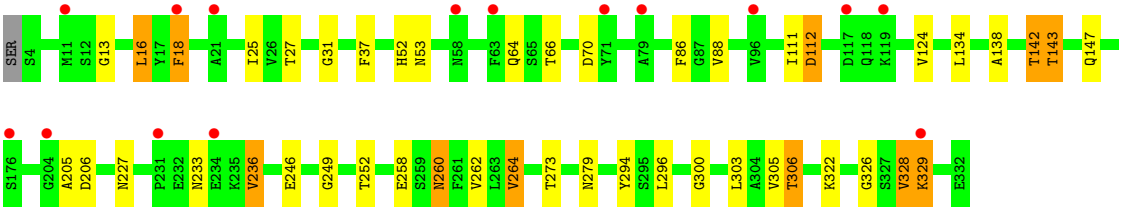
Chain AAA:



• Molecule 3: Lipoprotein

Chain DDD:




SER S4 M11 S12 G13 L16 Y17 F18 A21 I25 V26 T27 G31 F37 H52 N53 N58 F63 Q64 S65 T66 D70 Y71 A79 F86 G87 V88 V96 I111 D112 D117 Q118 K119 V124 L134 A138 T142 T143 Q147
S176 G204 A205 D206 N227 P231 E232 N233 E234 K235 V236 E246 G249 T252 E258 S259 N260 F261 V262 L263 V264 T273 N279 Y294 S295 L296 G300 L303 A304 V305 T306 K322 G326 S327 V328 K329 E332

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	78.02Å 304.31Å 128.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.30 49.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.09-2.30) 99.9 (49.09-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.250 0.214 , 0.253	Depositor DCC
R_{free} test set	3438 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10272	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, ACT, CAC, URI

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	BBB	0.69	0/2522	0.79	0/3406
1	CCC	0.71	0/2528	0.80	0/3414
2	AAA	0.71	0/2508	0.81	1/3387 (0.0%)
3	DDD	0.69	0/2505	0.79	1/3384 (0.0%)
All	All	0.70	0/10063	0.80	2/13591 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DDD	18	PHE	CB-CA-C	5.05	120.51	110.40
2	AAA	333	LYS	CA-C-O	-5.03	109.54	120.10

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	BBB	2477	0	2396	33	1
1	CCC	2483	0	2401	45	1
2	AAA	2466	0	2385	35	2
3	DDD	2463	0	2377	33	0
4	BBB	3	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CCC	2	0	0	0	1
4	DDD	4	0	0	0	2
5	AAA	17	0	12	0	0
5	BBB	17	0	12	0	0
5	CCC	17	0	12	0	0
5	DDD	17	0	12	0	0
6	CCC	5	0	0	1	0
7	BBB	8	0	6	3	0
8	AAA	84	0	0	5	0
8	BBB	87	0	0	5	0
8	CCC	102	0	0	4	1
8	DDD	20	0	0	0	1
All	All	10272	0	9613	141	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (141) 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:DDD:322:LYS:HB3	3:DDD:328:VAL:HG22	1.40	1.03
3:DDD:322:LYS:HB3	3:DDD:328:VAL:CG2	1.94	0.95
2:AAA:11:MET:CG	8:AAA:565:HOH:O	2.28	0.81
2:AAA:227:ASN:HD21	2:AAA:236:VAL:H	1.30	0.80
2:AAA:252:THR:HG22	2:AAA:258:GLU:HG3	1.63	0.79
3:DDD:227:ASN:HD21	3:DDD:236:VAL:H	1.31	0.77
1:CCC:227:ASN:HD21	1:CCC:236:VAL:H	1.32	0.77
2:AAA:11:MET:HG2	8:AAA:565:HOH:O	1.83	0.77
1:BBB:97:LYS:NZ	8:BBB:502:HOH:O	2.18	0.75
1:CCC:322:LYS:HB3	1:CCC:328:VAL:HG13	1.70	0.74
1:BBB:227:ASN:HD21	1:BBB:236:VAL:H	1.35	0.72
3:DDD:66:THR:HG22	3:DDD:70:ASP:OD2	1.91	0.71
3:DDD:322:LYS:CB	3:DDD:328:VAL:CG2	2.68	0.70
2:AAA:138:ALA:O	2:AAA:142:THR:HG23	1.93	0.69
1:BBB:138:ALA:O	1:BBB:142:THR:HG23	1.93	0.68
2:AAA:11:MET:HG3	8:AAA:565:HOH:O	1.92	0.68
1:CCC:164:ALA:HB2	1:CCC:333:LYS:C	2.13	0.68
3:DDD:138:ALA:O	3:DDD:142:THR:HG23	1.93	0.68
2:AAA:302:ASP:OD2	8:AAA:501:HOH:O	2.14	0.64
1:CCC:138:ALA:O	1:CCC:142:THR:HG23	1.96	0.64
3:DDD:246:GLU:HG3	3:DDD:306:THR:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:13:GLY:O	3:DDD:16:LEU:HD11	1.99	0.63
1:CCC:264:VAL:HG13	1:CCC:303:LEU:HD11	1.81	0.62
1:BBB:148:VAL:CG2	1:BBB:179:VAL:HG22	2.31	0.61
1:BBB:264:VAL:HG13	1:BBB:303:LEU:HD11	1.82	0.60
3:DDD:264:VAL:HG13	3:DDD:303:LEU:HD11	1.84	0.60
3:DDD:322:LYS:C	3:DDD:328:VAL:HG23	2.22	0.59
2:AAA:264:VAL:HG13	2:AAA:303:LEU:HD11	1.84	0.59
1:CCC:313:LYS:NZ	2:AAA:14:GLU:OE1	2.36	0.58
1:CCC:128:ASP:OD1	1:CCC:268:LYS:HD2	2.04	0.58
1:CCC:294:TYR:HB3	1:CCC:300:GLY:HA3	1.85	0.58
1:CCC:249:GLY:HA3	1:CCC:262:VAL:HG23	1.87	0.56
2:AAA:260:ASN:ND2	2:AAA:262:VAL:H	2.04	0.56
1:CCC:53:ASN:ND2	8:CCC:501:HOH:O	2.38	0.56
1:BBB:227:ASN:ND2	1:BBB:236:VAL:H	2.04	0.55
1:BBB:148:VAL:HG23	1:BBB:179:VAL:HG22	1.87	0.55
7:BBB:405:ACT:O	8:BBB:501:HOH:O	2.18	0.54
2:AAA:227:ASN:ND2	2:AAA:236:VAL:H	2.02	0.54
1:BBB:249:GLY:HA3	1:BBB:262:VAL:HG23	1.89	0.54
1:CCC:147:GLN:NE2	8:CCC:503:HOH:O	2.40	0.54
1:CCC:260:ASN:ND2	1:CCC:262:VAL:H	2.05	0.54
1:CCC:313:LYS:NZ	2:AAA:14:GLU:CD	2.62	0.53
3:DDD:227:ASN:ND2	3:DDD:236:VAL:H	2.01	0.53
2:AAA:294:TYR:HB3	2:AAA:300:GLY:HA3	1.90	0.53
1:BBB:260:ASN:ND2	1:BBB:262:VAL:H	2.07	0.53
1:BBB:231:PRO:HG2	1:BBB:234:GLU:HG3	1.90	0.53
1:CCC:134:LEU:HD11	1:CCC:296:LEU:HD21	1.91	0.52
1:BBB:161:ARG:NH1	8:BBB:505:HOH:O	2.37	0.52
3:DDD:260:ASN:ND2	3:DDD:262:VAL:H	2.06	0.52
1:CCC:31:GLY:CA	1:CCC:64:GLN:HE21	2.23	0.52
1:BBB:294:TYR:HB3	1:BBB:300:GLY:HA3	1.92	0.52
3:DDD:31:GLY:CA	3:DDD:64:GLN:HE21	2.23	0.52
3:DDD:326:GLY:O	3:DDD:329:LYS:HE3	2.09	0.52
2:AAA:233:ASN:HD22	2:AAA:234:GLU:HG3	1.75	0.51
1:CCC:53:ASN:HD21	2:AAA:244:ASP:HB3	1.76	0.51
1:BBB:68:GLU:HG2	8:BBB:569:HOH:O	2.09	0.51
1:BBB:31:GLY:CA	1:BBB:64:GLN:HE21	2.24	0.51
3:DDD:52:HIS:HE1	3:DDD:279:ASN:OD1	1.94	0.50
1:CCC:227:ASN:ND2	1:CCC:236:VAL:H	2.04	0.50
1:BBB:235:LYS:HE2	1:BBB:237:TRP:CH2	2.46	0.50
3:DDD:294:TYR:HB3	3:DDD:300:GLY:HA3	1.93	0.50
1:CCC:52:HIS:HE1	1:CCC:279:ASN:OD1	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:252:THR:HG22	3:DDD:258:GLU:HG2	1.92	0.50
1:CCC:260:ASN:HD22	1:CCC:262:VAL:H	1.60	0.49
1:BBB:246:GLU:HG3	1:BBB:306:THR:HG21	1.93	0.49
1:CCC:164:ALA:CB	1:CCC:333:LYS:C	2.79	0.49
2:AAA:29:THR:HG22	2:AAA:188:GLY:HA3	1.94	0.49
1:BBB:52:HIS:HE1	1:BBB:279:ASN:OD1	1.95	0.49
2:AAA:32:VAL:H	2:AAA:64:GLN:HE21	1.61	0.49
2:AAA:52:HIS:HE1	2:AAA:279:ASN:OD1	1.97	0.48
1:CCC:264:VAL:CG1	1:CCC:303:LEU:HD11	2.44	0.47
2:AAA:260:ASN:HD22	2:AAA:262:VAL:H	1.62	0.47
3:DDD:260:ASN:HD22	3:DDD:262:VAL:H	1.63	0.47
1:CCC:297:LYS:HG3	1:CCC:324:LEU:HD22	1.95	0.47
1:BBB:105:ASP:O	7:BBB:404:ACT:OXT	2.32	0.46
1:BBB:260:ASN:HD22	1:BBB:262:VAL:H	1.62	0.46
1:CCC:206:ASP:HA	1:CCC:236:VAL:HG22	1.97	0.46
1:CCC:305:VAL:HG11	1:CCC:313:LYS:CD	2.46	0.46
3:DDD:252:THR:HG22	3:DDD:258:GLU:CG	2.46	0.46
1:CCC:244:ASP:HB3	2:AAA:53:ASN:HD21	1.81	0.46
1:CCC:305:VAL:HG11	1:CCC:313:LYS:HG2	1.98	0.46
2:AAA:138:ALA:O	2:AAA:142:THR:CG2	2.62	0.46
1:BBB:138:ALA:O	1:BBB:142:THR:CG2	2.63	0.46
3:DDD:305:VAL:CG1	3:DDD:305:VAL:O	2.63	0.46
3:DDD:246:GLU:HG3	3:DDD:306:THR:CG2	2.46	0.45
2:AAA:325:ASP:OD1	2:AAA:326:GLY:N	2.50	0.45
1:CCC:25:ILE:HG22	1:CCC:86:PHE:HB2	1.99	0.45
1:BBB:105:ASP:O	7:BBB:404:ACT:C	2.65	0.45
1:BBB:134:LEU:HD11	1:BBB:296:LEU:HD21	1.99	0.45
2:AAA:264:VAL:CG1	2:AAA:303:LEU:HD11	2.47	0.45
1:BBB:25:ILE:HG22	1:BBB:86:PHE:HB2	1.99	0.44
3:DDD:138:ALA:O	3:DDD:142:THR:CG2	2.64	0.44
2:AAA:227:ASN:HD21	2:AAA:236:VAL:N	2.08	0.44
1:CCC:158:VAL:HG23	8:CCC:556:HOH:O	2.17	0.44
1:CCC:305:VAL:HG13	1:CCC:308:LEU:HB3	1.98	0.44
2:AAA:25:ILE:HG22	2:AAA:86:PHE:HB2	1.99	0.44
1:CCC:27:THR:HG21	1:CCC:64:GLN:HG3	2.00	0.44
1:CCC:147:GLN:O	1:CCC:205:ALA:HA	2.18	0.43
1:CCC:310:GLU:OE2	2:AAA:14:GLU:HB3	2.18	0.43
1:CCC:172:SER:O	6:CCC:404:CAC:AS	2.96	0.43
1:BBB:147:GLN:O	1:BBB:205:ALA:HA	2.18	0.43
1:BBB:264:VAL:CG1	1:BBB:303:LEU:HD11	2.46	0.43
3:DDD:25:ILE:HG22	3:DDD:86:PHE:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:147:GLN:O	3:DDD:205:ALA:HA	2.18	0.43
1:CCC:167:LYS:HE3	1:CCC:181:VAL:HG21	2.00	0.43
1:CCC:313:LYS:HZ2	2:AAA:14:GLU:CD	2.21	0.43
2:AAA:56:LYS:HE3	2:AAA:62:TYR:CE2	2.54	0.43
2:AAA:147:GLN:O	2:AAA:205:ALA:HA	2.18	0.43
1:CCC:37:PHE:CE2	1:CCC:88:VAL:HG12	2.53	0.43
1:CCC:227:ASN:HD21	1:CCC:236:VAL:N	2.09	0.43
1:BBB:174:ASP:HB3	1:BBB:177:ILE:HG13	2.01	0.43
2:AAA:143:THR:CG2	2:AAA:206:ASP:OD1	2.67	0.43
1:CCC:32:VAL:H	1:CCC:64:GLN:NE2	2.17	0.42
1:CCC:142:THR:HG21	1:CCC:263:LEU:HD11	2.01	0.42
1:CCC:138:ALA:O	1:CCC:142:THR:CG2	2.64	0.42
1:BBB:246:GLU:HG3	1:BBB:306:THR:CG2	2.48	0.42
1:CCC:124:VAL:HG11	1:CCC:273:THR:HG21	2.00	0.42
1:BBB:119:LYS:O	1:BBB:288:GLY:HA3	2.19	0.42
3:DDD:249:GLY:HA3	3:DDD:262:VAL:HG23	2.01	0.42
1:BBB:143:THR:CG2	1:BBB:206:ASP:OD1	2.67	0.42
1:CCC:20:GLY:HA2	1:CCC:282:GLU:CD	2.41	0.42
2:AAA:124:VAL:HG11	2:AAA:273:THR:HG21	2.01	0.42
1:BBB:52:HIS:CD2	1:BBB:282:GLU:OE2	2.73	0.42
3:DDD:134:LEU:HD11	3:DDD:296:LEU:HD21	2.01	0.42
1:CCC:227:ASN:HB3	1:CCC:251:TYR:CE2	2.55	0.41
3:DDD:143:THR:CG2	3:DDD:206:ASP:OD1	2.68	0.41
3:DDD:296:LEU:HD12	3:DDD:296:LEU:HA	1.96	0.41
3:DDD:326:GLY:O	3:DDD:329:LYS:CE	2.68	0.41
2:AAA:297:LYS:HG3	8:AAA:526:HOH:O	2.20	0.41
2:AAA:134:LEU:HD11	2:AAA:296:LEU:HD21	2.02	0.41
1:BBB:207:ILE:HG12	1:BBB:237:TRP:HB2	2.02	0.41
1:CCC:280:LYS:HE2	8:CCC:587:HOH:O	2.20	0.41
1:BBB:8:HIS:HD2	8:BBB:507:HOH:O	2.04	0.41
1:CCC:111:ILE:O	1:CCC:112:ASP:HB2	2.20	0.41
2:AAA:37:PHE:CE2	2:AAA:88:VAL:HG12	2.55	0.41
3:DDD:111:ILE:O	3:DDD:112:ASP:HB2	2.21	0.41
1:BBB:111:ILE:O	1:BBB:112:ASP:HB2	2.21	0.40
3:DDD:37:PHE:CE2	3:DDD:88:VAL:HG12	2.56	0.40
3:DDD:124:VAL:HG11	3:DDD:273:THR:HG21	2.03	0.40
3:DDD:264:VAL:CG1	3:DDD:303:LEU:HD11	2.49	0.40
2:AAA:111:ILE:O	2:AAA:112:ASP:HB2	2.20	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AAA:8:HIS:NE2	4:DDD:401:NI:NI[4_556]	1.35	0.85
1:BBB:282:GLU:OE2	4:CCC:402:NI:NI[6_445]	1.51	0.69
2:AAA:8:HIS:CE1	4:DDD:401:NI:NI[4_556]	1.56	0.64
1:CCC:282:GLU:OE2	4:BBB:402:NI:NI[6_444]	1.68	0.52
8:CCC:550:HOH:O	8:DDD:517:HOH:O[3_455]	2.18	0.02

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	BBB	329/331 (99%)	316 (96%)	11 (3%)	2 (1%)	25	31
1	CCC	330/331 (100%)	315 (96%)	14 (4%)	1 (0%)	41	50
2	AAA	327/329 (99%)	309 (94%)	16 (5%)	2 (1%)	25	31
3	DDD	327/330 (99%)	311 (95%)	14 (4%)	2 (1%)	25	31
All	All	1313/1321 (99%)	1251 (95%)	55 (4%)	7 (0%)	29	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AAA	306	THR
1	BBB	306	THR
3	DDD	306	THR
1	BBB	112	ASP
1	CCC	112	ASP
2	AAA	112	ASP
3	DDD	112	ASP

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	BBB	255/255 (100%)	234 (92%)	21 (8%)	11	14
1	CCC	256/255 (100%)	238 (93%)	18 (7%)	15	19
2	AAA	253/253 (100%)	238 (94%)	15 (6%)	19	27
3	DDD	253/254 (100%)	241 (95%)	12 (5%)	26	37
All	All	1017/1017 (100%)	951 (94%)	66 (6%)	17	23

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	16	LEU
1	CCC	27	THR
1	CCC	142	THR
1	CCC	143	THR
1	CCC	144	LYS
1	CCC	176	SER
1	CCC	177	ILE
1	CCC	225	SER
1	CCC	236	VAL
1	CCC	252	THR
1	CCC	254	LYS
1	CCC	259	SER
1	CCC	260	ASN
1	CCC	264	VAL
1	CCC	297	LYS
1	CCC	311	GLU
1	CCC	314	LYS
1	CCC	329	LYS
2	AAA	7	HIS
2	AAA	19	GLN
2	AAA	27	THR
2	AAA	77	GLN
2	AAA	97	LYS
2	AAA	102	GLU
2	AAA	142	THR
2	AAA	143	THR
2	AAA	194	LYS
2	AAA	233	ASN
2	AAA	236	VAL
2	AAA	260	ASN

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Mol	Chain	Res	Type
2	AAA	264	VAL
2	AAA	310	GLU
2	AAA	317	GLU
1	BBB	5	HIS
1	BBB	16	LEU
1	BBB	27	THR
1	BBB	97	LYS
1	BBB	116	LYS
1	BBB	142	THR
1	BBB	143	THR
1	BBB	177	ILE
1	BBB	178	LYS
1	BBB	225	SER
1	BBB	230	ARG
1	BBB	233	ASN
1	BBB	235	LYS
1	BBB	236	VAL
1	BBB	246	GLU
1	BBB	252	THR
1	BBB	260	ASN
1	BBB	264	VAL
1	BBB	310	GLU
1	BBB	317	GLU
1	BBB	327	SER
3	DDD	16	LEU
3	DDD	18	PHE
3	DDD	27	THR
3	DDD	53	ASN
3	DDD	142	THR
3	DDD	143	THR
3	DDD	233	ASN
3	DDD	236	VAL
3	DDD	260	ASN
3	DDD	264	VAL
3	DDD	328	VAL
3	DDD	329	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	CAC	CCC	404	-	0,4,4	-	-	0,6,6	-	-
5	URI	DDD	402	-	18,18,18	0.30	0	26,26,26	0.51	0
7	ACT	BBB	404	-	3,3,3	0.91	0	3,3,3	0.97	0
7	ACT	BBB	405	-	3,3,3	1.04	0	3,3,3	0.75	0
5	URI	CCC	403	-	18,18,18	0.22	0	26,26,26	0.52	0
5	URI	BBB	403	-	18,18,18	0.38	0	26,26,26	0.43	0
5	URI	AAA	401	-	18,18,18	0.30	0	26,26,26	0.54	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
5	URI	CCC	403	-	-	0/6/22/22	0/2/2/2
5	URI	AAA	401	-	-	0/6/22/22	0/2/2/2
5	URI	DDD	402	-	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	URI	BBB	403	-	-	0/6/22/22	0/2/2/2

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	CCC	404	CAC	1	0
7	BBB	404	ACT	2	0
7	BBB	405	ACT	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, 95^{th} 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	BBB	330/331 (99%)	-0.01	3 (0%)	84	88	29, 49, 89, 107	0
1	CCC	331/331 (100%)	-0.13	2 (0%)	89	92	27, 46, 81, 106	0
2	AAA	329/329 (100%)	-0.03	5 (1%)	73	79	27, 50, 81, 137	0
3	DDD	329/330 (99%)	0.36	15 (4%)	32	39	47, 73, 109, 122	0
All	All	1319/1321 (99%)	0.05	25 (1%)	66	73	27, 54, 97, 137	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	AAA	16	LEU	4.1
1	BBB	204	GLY	3.8
3	DDD	63	PHE	3.4
3	DDD	117	ASP	2.8
2	AAA	7	HIS	2.7
1	BBB	231	PRO	2.7
1	CCC	333	LYS	2.6
3	DDD	21	ALA	2.6
3	DDD	119	LYS	2.6
3	DDD	11	MET	2.5
1	BBB	333	LYS	2.5
2	AAA	17	TYR	2.5
2	AAA	79	ALA	2.4
3	DDD	96	VAL	2.4
3	DDD	71	TYR	2.3
3	DDD	234	GLU	2.3
3	DDD	176	SER	2.3
3	DDD	79	ALA	2.2
3	DDD	58	ASN	2.2
1	CCC	256	GLY	2.2
3	DDD	329	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	DDD	231	PRO	2.1
3	DDD	204	GLY	2.0
2	AAA	254	LYS	2.0
3	DDD	18	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
6	CAC	CCC	404	5/5	0.82	0.14	144,147,154,166	0
7	ACT	BBB	405	4/4	0.84	0.18	77,78,80,87	0
7	ACT	BBB	404	4/4	0.87	0.15	65,70,71,77	0
4	NI	BBB	401	1/1	0.90	0.09	82,82,82,82	0
4	NI	DDD	404	1/1	0.94	0.06	78,78,78,78	0
4	NI	DDD	403	1/1	0.95	0.21	59,59,59,59	0
5	URI	DDD	402	17/17	0.96	0.11	46,50,54,56	0
4	NI	DDD	401	1/1	0.97	0.08	59,59,59,59	0
4	NI	BBB	402	1/1	0.98	0.15	30,30,30,30	0
5	URI	CCC	403	17/17	0.98	0.10	30,33,38,38	0
5	URI	AAA	401	17/17	0.98	0.10	29,35,39,40	0
5	URI	BBB	403	17/17	0.98	0.12	33,36,39,42	0
4	NI	DDD	405	1/1	0.99	0.07	44,44,44,44	0
4	NI	CCC	402	1/1	0.99	0.14	31,31,31,31	0
4	NI	BBB	406	1/1	1.00	0.08	97,97,97,97	0
4	NI	CCC	401	1/1	1.00	0.11	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.