Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2014 – 05:12 PM EDT

PDB ID	:	4CCL
Title	:	X-Ray structure of E. coli ycfD
Authors	:	McDonough, M.A.; Ho, C.H.; Kershaw, N.J.; Schofield, C.J.
Deposited on	:	2013-10-23
Resolution	:	2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html
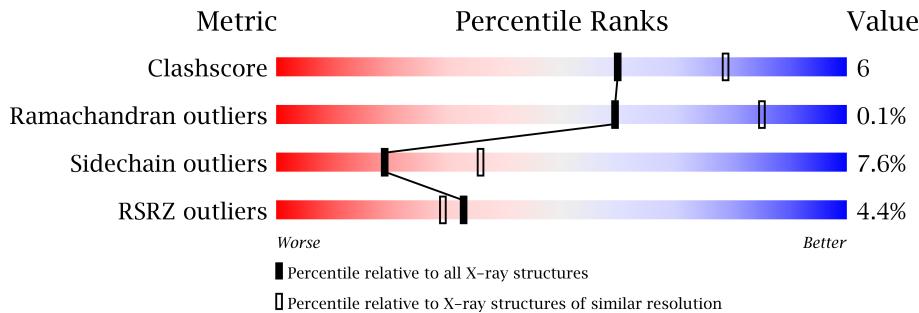
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23161
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23161

1 Overall quality at a glance ⓘ
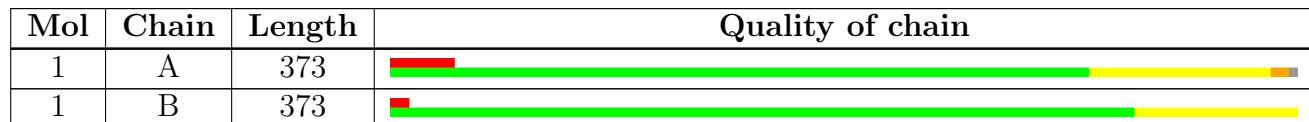
The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		7.6%
RSRZ outliers		4.4%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	B	1378	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6087 atoms, of which 0 are hydrogen and 0 are deuterium.

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.
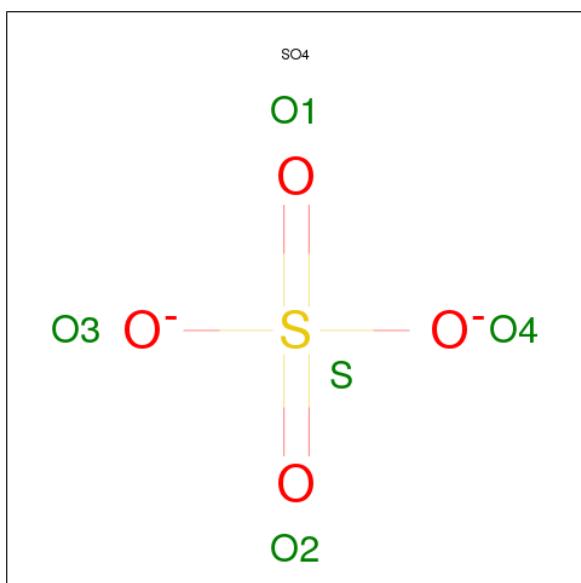
- Molecule 1 is a protein called 50S RIBOSOMAL PROTEIN L16 ARGININE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	371	Total 2907	C 1865	N 494	O 539	S 1	Se 8	0	0	0
1	B	372	Total 2976	C 1906	N 507	O 552	S 1	Se 10	0	1	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mn 2	0	0
2	A	2	Total 2	Mn 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
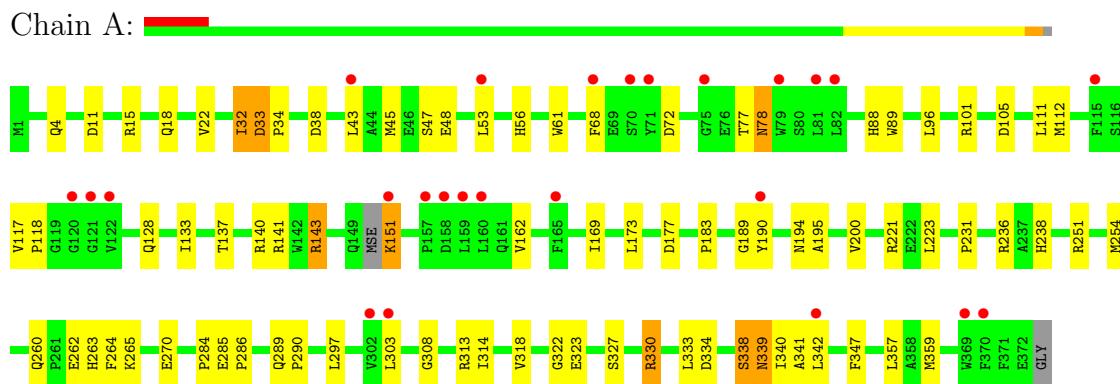
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	100	Total 100	O 100	0	0
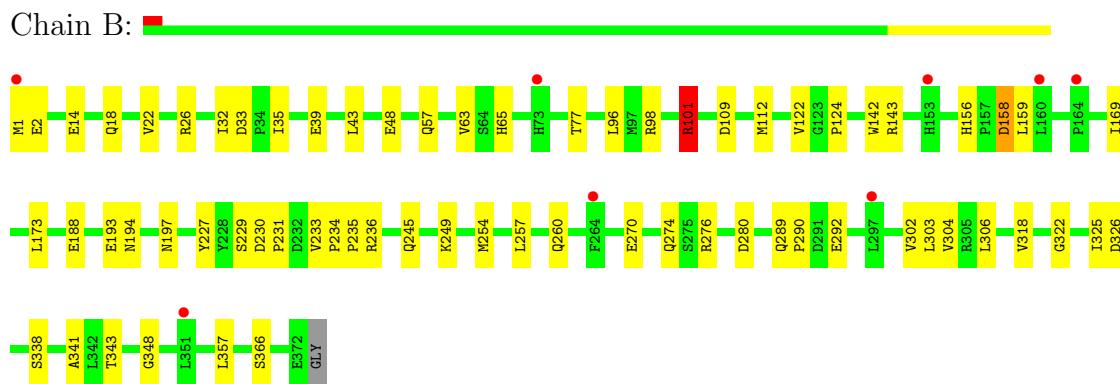
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 (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: 50S RIBOSOMAL PROTEIN L16 ARGININE HYDROXYLASE

Chain A:

• Molecule 1: 50S RIBOSOMAL PROTEIN L16 ARGININE HYDROXYLASE

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.69Å 120.69Å 133.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.77 – 2.60 44.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.77-2.60) 92.7 (44.76-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.249 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 30988 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6087	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5   Model quality   ⓘ

5.1   Standard geometry   ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.27	0/2987	0.53	0/4064
1	B	0.25	0/3063	0.50	1/4163 (0.0%)
All	All	0.26	0/6050	0.51	1/8227 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2907	0	2703	42	0
1	B	2976	0	2808	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	25	0	0	0	0
3	B	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	55	0	0	1	0
4	B	100	0	0	1	0
All	All	6087	0	5511	69	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (69) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:156:HIS:HD2	1:B:158:ASP:H	1.39	0.69
1:B:348:GLY:O	4:B:2100:HOH:O	2.09	0.69
1:B:63:VAL:HG21	1:B:159:LEU:HB2	1.81	0.62
1:A:77:THR:HG23	1:A:78:ASN:HB2	1.85	0.59
1:A:251:ARG:HA	1:A:254:MSE:HE2	1.85	0.58
1:A:48:GLU:HG3	1:A:89:TRP:CH2	2.39	0.57
1:A:303:LEU:O	1:A:341:ALA:HA	2.05	0.56
1:A:264:PHE:CE1	1:B:254:MSE:HE1	2.41	0.56
1:A:327:SER:HB3	1:A:333:LEU:HD11	1.89	0.55
1:A:339:ASN:HB2	1:A:342:LEU:HD13	1.89	0.54
1:A:327:SER:HB2	1:A:359:MSE:SE	2.58	0.54
1:B:1:MSE:O	1:B:98:ARG:NH2	2.41	0.53
1:A:140:ARG:HH21	1:A:190:TYR:HA	1.76	0.51
1:B:143:ARG:HA	1:B:169:ILE:O	2.11	0.51
1:A:265:LYS:HE3	1:A:314:ILE:HG22	1.93	0.51
1:A:223:LEU:HD13	1:A:263:HIS:CD2	2.46	0.49
1:B:156:HIS:CD2	1:B:158:ASP:H	2.25	0.49
1:A:330:ARG:HD2	1:A:330:ARG:H	1.76	0.49
1:B:229:SER:O	1:B:249:LYS:NZ	2.31	0.49
1:A:231:PRO:HA	1:B:18:GLN:HB2	1.95	0.49
1:B:101:ARG:HH11	1:B:101:ARG:CG	2.26	0.49
1:B:304:VAL:HG12	1:B:341:ALA:HA	1.95	0.48
1:A:88:HIS:CD2	1:A:308:GLY:HA3	2.48	0.48
1:A:334:ASP:O	1:A:338:SER:HB2	2.13	0.48
1:B:280:ASP:O	1:B:306:LEU:HD11	2.14	0.47
1:A:137:THR:O	1:A:195:ALA:HA	2.15	0.47
1:B:234:PRO:HA	1:B:235:PRO:HD3	1.83	0.47
1:A:101:ARG:NH1	1:A:105:ASP:OD2	2.48	0.46
1:A:151:LYS:HB2	1:A:151:LYS:HE3	1.66	0.46
1:A:56:HIS:HB3	1:A:61:TRP:CE3	2.50	0.45
1:A:11:ASP:OD2	1:A:15:ARG:NH1	2.49	0.45
1:A:128:GLN:HG2	1:B:227:TYR:CE1	2.51	0.45
1:B:257:LEU:HA	1:B:260:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1:MSE:HG2	1:B:2:GLU:H	1.82	0.45
1:A:330:ARG:HD2	1:A:330:ARG:N	2.32	0.45
1:B:318:VAL:HB	1:B:325:ILE:HG13	1.99	0.44
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.83	0.44
1:A:118:PRO:HD3	1:A:194:ASN:OD1	2.17	0.44
1:A:318:VAL:HG21	1:A:333:LEU:HB3	1.99	0.44
1:B:290:PRO:HB3	1:B:357:LEU:HG	1.99	0.44
1:B:35:ILE:HG12	1:B:39:GLU:HB2	1.99	0.44
1:A:284:PRO:HB2	1:A:286:PRO:O	2.18	0.44
1:A:96:LEU:HD23	1:A:111:LEU:HD11	2.00	0.43
1:B:193[B]:GLU:HG2	1:B:194:ASN:N	2.34	0.43
1:A:143:ARG:HA	1:A:169:ILE:O	2.19	0.43
1:B:270:GLU:O	1:B:322:GLY:HA2	2.19	0.43
1:A:173:LEU:HG	1:A:177:ASP:HB3	2.00	0.43
1:A:297:LEU:HD21	1:A:347:PHE:CE2	2.54	0.43
1:A:18:GLN:HB2	1:B:231:PRO:HA	2.01	0.42
1:B:289:GLN:O	1:B:292:GLU:HG2	2.19	0.42
1:A:141:ARG:O	1:A:189:GLY:HA2	2.20	0.42
1:A:32:ILE:O	1:A:32:ILE:HG13	2.18	0.42
1:B:124:PRO:HA	1:B:188:GLU:HB2	2.02	0.42
1:B:1:MSE:HE1	1:B:32:ILE:HD12	2.01	0.42
1:B:230:ASP:HB2	1:B:233:VAL:HB	2.02	0.41
1:A:33:ASP:HA	1:A:34:PRO:HD3	1.88	0.41
1:A:128:GLN:C	1:A:183:PRO:HB3	2.41	0.41
4:A:2013:HOH:O	1:B:236:ARG:NH1	2.53	0.41
1:A:290:PRO:HB3	1:A:357:LEU:HD13	2.03	0.41
1:A:45:MSE:HB3	1:A:68:PHE:O	2.21	0.41
1:A:260:GLN:HG2	1:A:263:HIS:CD2	2.56	0.41
1:A:289:GLN:HG3	1:A:290:PRO:HD2	2.02	0.41
1:B:109:ASP:OD2	1:B:276:ARG:NH1	2.54	0.41
1:A:270:GLU:O	1:A:322:GLY:HA2	2.19	0.41
1:B:193[B]:GLU:HG2	1:B:194:ASN:H	1.86	0.41
1:A:238:HIS:HB3	1:B:338:SER:OG	2.20	0.40
1:B:142:TRP:CD1	1:B:173:LEU:HD22	2.56	0.40
1:B:96:LEU:HD23	1:B:96:LEU:HA	1.92	0.40
1:A:68:PHE:HA	1:A:68:PHE:HD1	1.81	0.40

There are no symmetry-related clashes.

5.3   Torsion angles

5.3.1   Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	367/373 (98%)	347 (95%)	19 (5%)	1 (0%)	50	77
1	B	371/373 (100%)	360 (97%)	11 (3%)	0	100	100
All	All	738/746 (99%)	707 (96%)	30 (4%)	1 (0%)	59	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	VAL

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	294/311 (94%)	269 (92%)	25 (8%)	15	29
1	B	312/311 (100%)	291 (93%)	21 (7%)	23	44
All	All	606/622 (97%)	560 (92%)	46 (8%)	19	36

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	22	VAL
1	A	32	ILE
1	A	33	ASP
1	A	38	ASP
1	A	47	SER
1	A	53	LEU
1	A	72	ASP

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	112	MSE
1	A	117	VAL
1	A	133	ILE
1	A	143	ARG
1	A	151	LYS
1	A	200	VAL
1	A	221	ARG
1	A	236	ARG
1	A	262	GLU
1	A	285	GLU
1	A	313	ARG
1	A	323	GLU
1	A	330	ARG
1	A	338	SER
1	A	339	ASN
1	A	340	ILE
1	B	14	GLU
1	B	22	VAL
1	B	26	ARG
1	B	33	ASP
1	B	43	LEU
1	B	48	GLU
1	B	57	GLN
1	B	65	HIS
1	B	77	THR
1	B	101	ARG
1	B	112	MSE
1	B	122	VAL
1	B	158	ASP
1	B	197	ASN
1	B	245	GLN
1	B	274	GLN
1	B	302	VAL
1	B	303	LEU
1	B	326	ASP
1	B	343	THR
1	B	366	SER

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

Mol	Chain	Res	Type
1	A	16	HIS
1	A	263	HIS
1	B	156	HIS
1	B	274	GLN

5.3.3   RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5   Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6   Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7   Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.8   Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	371/373 (99%)	0.47	25 (6%)	17	15	52, 88, 142, 168	0
1	B	372/373 (99%)	0.20	8 (2%)	59	56	41, 69, 113, 155	0
All	All	743/746 (99%)	0.34	33 (4%)	33	29	41, 76, 129, 168	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	TYR	5.3
1	A	70	SER	4.4
1	A	79	TRP	4.2
1	A	122	VAL	4.0
1	A	68	PHE	3.6
1	B	160	LEU	3.6
1	A	190	TYR	3.1
1	A	81	LEU	3.1
1	A	158	ASP	3.0
1	A	302	VAL	2.9
1	A	369	TRP	2.9
1	A	160	LEU	2.9
1	A	120	GLY	2.9
1	A	121	GLY	2.7
1	A	43	LEU	2.6
1	A	157	PRO	2.6
1	A	82	LEU	2.6
1	B	1	MSE	2.4
1	B	164	PRO	2.4
1	A	159	LEU	2.4
1	A	53	LEU	2.4
1	B	73	HIS	2.4
1	A	75	GLY	2.3
1	B	297	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	165	PHE	2.2
1	A	342	LEU	2.2
1	A	303	LEU	2.1
1	A	115	PHE	2.1
1	B	264	PHE	2.1
1	B	351	LEU	2.0
1	A	151	LYS	2.0
1	B	153	HIS	2.0
1	A	370	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	B	1378	5/5	0.32	4.89	194,195,196,196	0
3	SO4	A	1375	5/5	0.34	1.49	134,139,141,143	0
2	MN	A	1374	1/1	0.21	1.08	153,153,153,153	0
3	SO4	A	1379	5/5	0.17	0.62	165,166,166,168	0
3	SO4	A	1377	5/5	0.17	0.61	107,115,120,122	0
3	SO4	A	1376	5/5	0.17	-0.27	161,164,165,166	0
2	MN	B	1373	1/1	0.11	-0.51	112,112,112,112	0
3	SO4	A	1378	5/5	0.16	-0.76	136,138,141,142	0
3	SO4	B	1376	5/5	0.14	-1.49	81,88,95,100	0
3	SO4	B	1377	5/5	0.17	-1.54	153,154,156,158	0
3	SO4	B	1375	5/5	0.11	-2.01	62,65,74,75	0
2	MN	B	1374	1/1	0.08	-2.18	107,107,107,107	0
2	MN	A	1373	1/1	0.07	-3.23	104,104,104,104	1

6.5 Other polymers (i)

There are no such residues in this entry.