W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Apr 1, 2025 – 10:15 pm BST

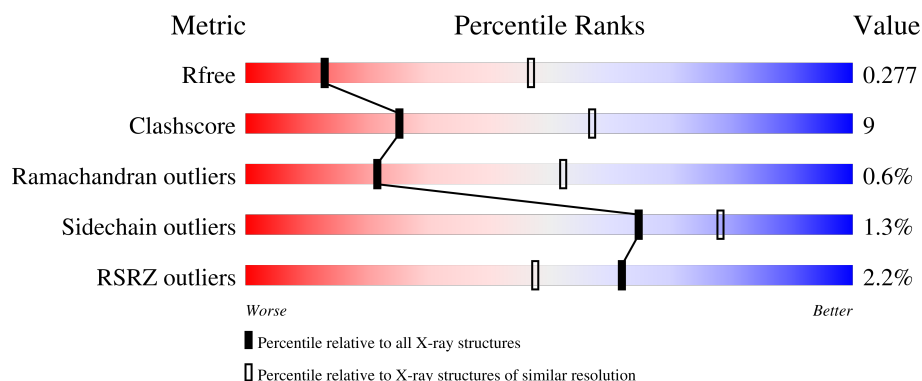|		
PDB ID	:	5O5Q / pdb_00005o5q
Title	:	X-ray crystal structure of RapZ from Escherichia coli (P3221 space group)
Authors	:	Gonzalez, G.M.; Durica-Mitic, S.; Hardwick, S.W.; Moncrieffe, M.; Resch, M.; Neumann, P.; Ficner, R.; Gorke, B.; Luisi, B.F.
Deposited on	:	2017-06-02
Resolution	:	3.25 Å(reported)

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 3.25 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
Rfree		0.277
Clashscore		9
Ramachandran outliers		0.6%
Sidechain outliers		1.3%
RSRZ outliers		2.2%

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))
R_{free}	164625	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (3.30-3.22)

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	A	295	74% 16% 10%
1	B	295	.% / 70% 21% • 8%
1	C	295	4% / 67% 18% • 14%
1	D	295	3% / 72% 20% • 6%

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
2	SO4	B	302	-	-	X	-
2	SO4	B	303	-	-	X	-
2	SO4	C	301	-	-	X	-
2	SO4	D	301	-	-	X	-
2	SO4	D	302	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8160 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 RNase adapter protein RapZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2051	1303	350	387	11			
1	B	272	Total	C	N	O	S	3	0	0
			2102	1324	368	400	10			
1	D	276	Total	C	N	O	S	0	0	0
			2102	1326	364	400	12			
1	C	254	Total	C	N	O	S	0	0	0
			1828	1156	314	349	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P0A894
A	-9	TRP	-	expression tag	UNP P0A894
A	-8	SER	-	expression tag	UNP P0A894
A	-7	HIS	-	expression tag	UNP P0A894
A	-6	PRO	-	expression tag	UNP P0A894
A	-5	GLN	-	expression tag	UNP P0A894
A	-4	PHE	-	expression tag	UNP P0A894
A	-3	GLU	-	expression tag	UNP P0A894
A	-2	LYS	-	expression tag	UNP P0A894
A	-1	ALA	-	expression tag	UNP P0A894
A	0	SER	-	expression tag	UNP P0A894
B	-10	MET	-	initiating methionine	UNP P0A894
B	-9	TRP	-	expression tag	UNP P0A894
B	-8	SER	-	expression tag	UNP P0A894
B	-7	HIS	-	expression tag	UNP P0A894
B	-6	PRO	-	expression tag	UNP P0A894
B	-5	GLN	-	expression tag	UNP P0A894
B	-4	PHE	-	expression tag	UNP P0A894
B	-3	GLU	-	expression tag	UNP P0A894
B	-2	LYS	-	expression tag	UNP P0A894
B	-1	ALA	-	expression tag	UNP P0A894

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P0A894
D	-10	MET	-	initiating methionine	UNP P0A894
D	-9	TRP	-	expression tag	UNP P0A894
D	-8	SER	-	expression tag	UNP P0A894
D	-7	HIS	-	expression tag	UNP P0A894
D	-6	PRO	-	expression tag	UNP P0A894
D	-5	GLN	-	expression tag	UNP P0A894
D	-4	PHE	-	expression tag	UNP P0A894
D	-3	GLU	-	expression tag	UNP P0A894
D	-2	LYS	-	expression tag	UNP P0A894
D	-1	ALA	-	expression tag	UNP P0A894
D	0	SER	-	expression tag	UNP P0A894
C	-10	MET	-	initiating methionine	UNP P0A894
C	-9	TRP	-	expression tag	UNP P0A894
C	-8	SER	-	expression tag	UNP P0A894
C	-7	HIS	-	expression tag	UNP P0A894
C	-6	PRO	-	expression tag	UNP P0A894
C	-5	GLN	-	expression tag	UNP P0A894
C	-4	PHE	-	expression tag	UNP P0A894
C	-3	GLU	-	expression tag	UNP P0A894
C	-2	LYS	-	expression tag	UNP P0A894
C	-1	ALA	-	expression tag	UNP P0A894
C	0	SER	-	expression tag	UNP P0A894

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	C	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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.
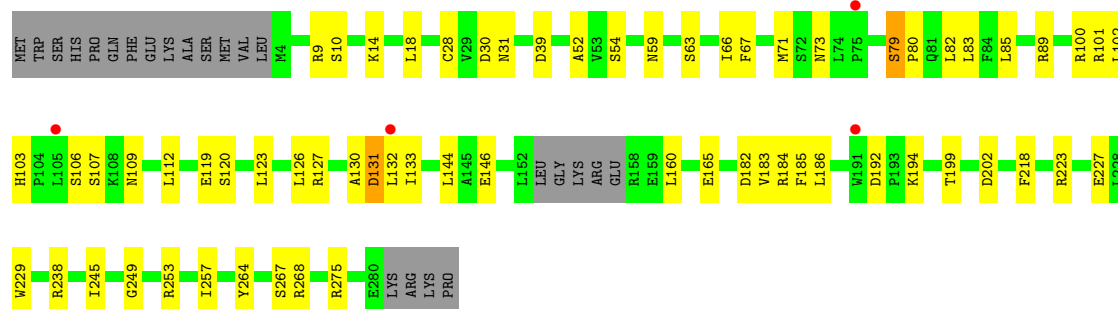
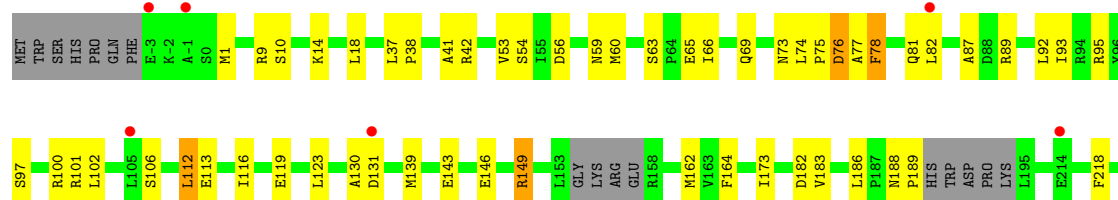• Molecule 1: RNase adapter protein RapZ

Chain A:
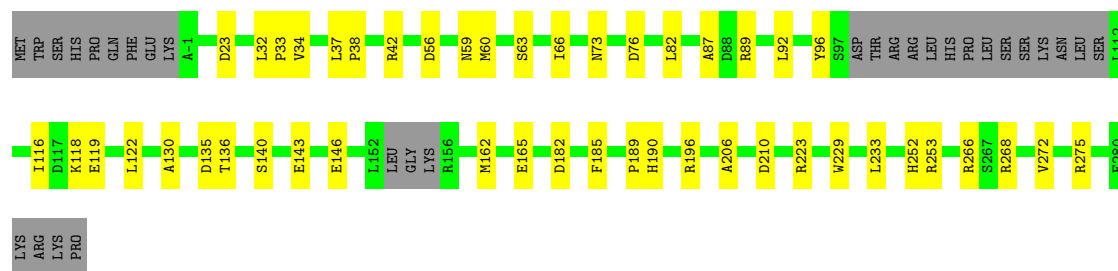
• Molecule 1: RNase adapter protein RapZ

Chain B:

• Molecule 1: RNase adapter protein RapZ

Chain D:

E227 N236 N237 V243 H252 Y264 F265 R268 V272 K281 ARG LYS PRO

● Molecule 1: RNase adapter protein RapZ

Chain C:

4%

67%										18%		●		14%

MET TRP SER HIS PRO GLN PHE GLU LYS ALA SER M1 V2 L3 M4 I5 S15 L18 R19 M24 C28 V35 L36 L37 P38 A41 A45 D46 S50 V53 N59 MET PRO GLU S63 P64 F67 E68 N73 D76 A77 F78 L82 L83 F84 L85

D86 ALA D88 Y96 SER ASP THR ARG ARG LEU HIS PRO LEU SER SER LYS ASN LEU SER LEU E113 E124 P125 R129 A130 D131 V134 D135 THR SER GLU MET SER VAL HIS E143 L144 A145 E146 M147 T150 R151 L152 L153 G154 K155 ARG E157 L160 T161 M162 K170 H171

G172 I173 V183 L186 P189 H190 W191 R196 L201 D210 H216 R223 W229 M232 N237 R238 G249 R253 E259 Y264 R268 V272 R282 LYS PRO

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.54Å 91.54Å 352.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.77 – 3.25 45.77 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.77-3.25) 97.6 (45.77-3.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.25Å)	Xtriage
Refinement program	PHENIX (dev_2747: ???)	Depositor
R, R_{free}	0.218 , 0.273 0.219 , 0.277	Depositor DCC
R_{free} test set	1372 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	96.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 111.6	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8160	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 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	0.28	0/2092	0.49	0/2842
1	B	0.28	0/2145	0.51	0/2913
1	C	0.26	0/1862	0.48	0/2540
1	D	0.27	0/2141	0.48	0/2908
All	All	0.27	0/8240	0.49	0/11203

There are no bond length outliers.

There are no bond angle outliers.

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	2051	0	1995	29	0
1	B	2102	0	2022	52	0
1	C	1828	0	1630	38	0
1	D	2102	0	2007	43	0
2	A	20	0	0	1	0
2	B	15	0	0	7	0
2	C	10	0	0	3	0
2	D	30	0	0	8	0
3	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
All	All	8160	0	7654	150	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.

The worst 5 of 150 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)
1:C:162:MET:HB2	1:C:272:VAL:HG12	1.63	0.81
1:A:182:ASP:OD2	1:B:238:ARG:NH2	2.15	0.79
1:A:266:ARG:NH2	3:A:401:HOH:O	2.18	0.75
1:B:82:LEU:HD11	1:B:126:LEU:HD21	1.71	0.73
1:D:14:LYS:NZ	2:D:302:SO4:O3	2.23	0.72

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	259/295 (88%)	252 (97%)	7 (3%)	0	100	100
1	B	268/295 (91%)	253 (94%)	14 (5%)	1 (0%)	30	60
1	C	242/295 (82%)	226 (93%)	12 (5%)	4 (2%)	7	30
1	D	270/295 (92%)	257 (95%)	12 (4%)	1 (0%)	30	60
All	All	1039/1180 (88%)	988 (95%)	45 (4%)	6 (1%)	22	52

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	SER

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Mol	Chain	Res	Type
1	D	76	ASP
1	C	124	GLU
1	C	190	HIS
1	C	134	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	220/264 (83%)	218 (99%)	2 (1%)	75	84
1	B	225/264 (85%)	221 (98%)	4 (2%)	54	72
1	C	172/264 (65%)	171 (99%)	1 (1%)	84	89
1	D	220/264 (83%)	216 (98%)	4 (2%)	54	72
All	All	837/1056 (79%)	826 (99%)	11 (1%)	65	78

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	78	PHE
1	D	112	LEU
1	C	1	MET
1	D	149	ARG
1	B	131	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	B	73	ASN
1	D	31	ASN
1	C	73	ASN
1	C	171	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

15 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	B	301	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	D	303	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	B	302	-	4,4,4	0.21	0	6,6,6	0.15	0
2	SO4	D	305	1	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	D	306	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	A	304	1	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	301	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	302	1	4,4,4	0.11	0	6,6,6	0.17	0
2	SO4	D	302	-	4,4,4	0.11	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	SO4	1	0
2	D	301	SO4	3	0
2	D	303	SO4	1	0
2	B	302	SO4	4	0
2	B	303	SO4	2	0
2	A	302	SO4	1	0
2	C	301	SO4	2	0
2	D	304	SO4	1	0
2	C	302	SO4	1	0
2	D	302	SO4	3	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(Å²)	Q<0.9
1	A	265/295 (89%)	-0.26	0	100	100	48, 99, 164, 243	1 (0%)
1	B	272/295 (92%)	-0.18	4 (1%)	71	58	57, 111, 189, 255	1 (0%)
1	C	254/295 (86%)	-0.06	11 (4%)	40	30	60, 127, 233, 310	0
1	D	276/295 (93%)	-0.08	9 (3%)	49	36	57, 108, 186, 236	0
All	All	1067/1180 (90%)	-0.15	24 (2%)	62	48	48, 108, 200, 310	2 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	131	ASP	4.6
1	C	24	MET	3.8
1	D	214	GLU	3.5
1	C	4	MET	3.3
1	C	83	LEU	3.2

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 monosaccharides 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. 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.

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PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	304	5/5	0.46	0.12	190,236,306,306	0
2	SO4	C	301	5/5	0.75	0.10	122,127,140,140	0
2	SO4	A	303	5/5	0.77	0.18	255,256,259,262	0
2	SO4	D	306	5/5	0.78	0.16	225,229,244,247	0
2	SO4	D	305	5/5	0.79	0.12	192,210,215,215	0
2	SO4	A	302	5/5	0.80	0.10	130,139,142,145	0
2	SO4	B	303	5/5	0.82	0.08	126,128,150,159	0
2	SO4	C	302	5/5	0.84	0.07	158,227,230,262	0
2	SO4	D	304	5/5	0.85	0.14	118,119,133,139	0
2	SO4	D	303	5/5	0.90	0.15	128,138,140,143	0
2	SO4	B	301	5/5	0.92	0.09	94,95,103,122	0
2	SO4	B	302	5/5	0.95	0.07	48,69,88,96	0
2	SO4	A	301	5/5	0.96	0.05	82,85,106,115	0
2	SO4	D	301	5/5	0.96	0.07	66,76,90,95	0
2	SO4	D	302	5/5	0.97	0.06	57,70,77,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.