



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:14 AM GMT

PDB ID : 3F1R  
Title : Crystal structure of FGF20 dimer  
Authors : Kalinina, J.; Mohammadi, M.  
Deposited on : 2008-10-28  
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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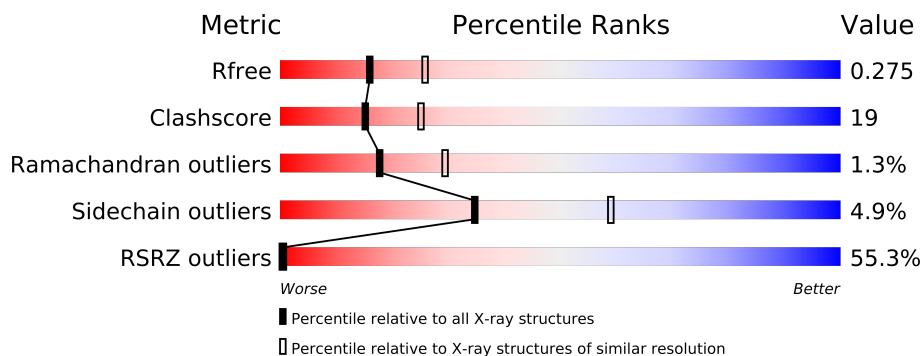
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	211	
1	B	211	

## 2 Entry composition i

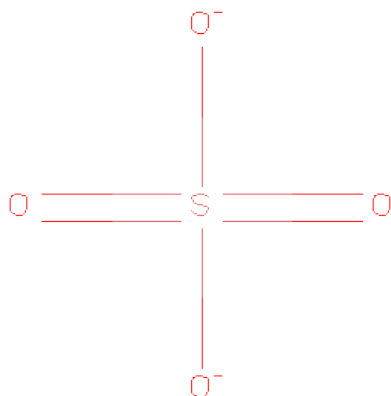
There are 3 unique types of molecules in this entry. The entry contains 2549 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Fibroblast growth factor 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1257	796	229	229	3			
1	B	157	Total	C	N	O	S	0	0	0
			1253	794	229	227	3			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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

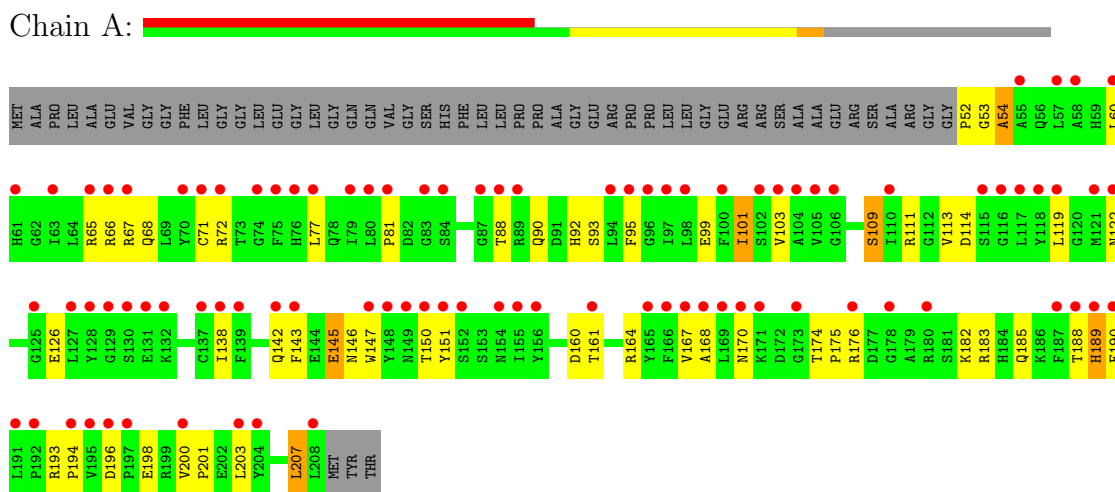
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	3	Total	O	0	0
			3	3		

### 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: Fibroblast growth factor 20



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.14Å 102.14Å 119.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.58 – 2.50 35.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.58-2.50) 88.8 (35.58-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.67 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.256 , 0.273 0.276 , 0.275	Depositor DCC
$R_{free}$ test set	680 reflections (4.75%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	1.419	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 73.0	EDS
Estimated twinning fraction	0.021 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.000 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.000 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.000 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.021 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.490 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 16050 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	2549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>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: 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	0.44	0/1287	0.69	1/1736 (0.1%)
1	B	0.45	0/1283	0.68	1/1731 (0.1%)
All	All	0.44	0/2570	0.69	2/3467 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1052	PRO	N-CA-CB	5.50	109.90	103.30
1	A	52	PRO	N-CA-CB	5.43	109.82	103.30

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	1257	0	1221	43	0
1	B	1253	0	1217	53	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	6	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	1	0
All	All	2549	0	2438	94	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 19.

All (94) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1097:ILE:HD11	1:B:1200:VAL:HG11	1.52	0.92
1:A:164:ARG:HB3	3:A:2004:HOH:O	1.72	0.90
1:A:196:ASP:HB3	1:A:198:GLU:OE2	1.71	0.89
1:B:1113:VAL:HG12	1:B:1203:LEU:HD22	1.59	0.84
1:A:207:LEU:HD23	1:A:207:LEU:H	1.47	0.77
1:A:101:ILE:HG13	1:A:101:ILE:O	1.86	0.74
1:A:122:ASN:ND2	1:A:126:GLU:HG3	2.06	0.71
1:A:122:ASN:HD21	1:A:126:GLU:HG3	1.56	0.70
1:B:1196:ASP:HB3	1:B:1198:GLU:OE2	1.91	0.70
1:B:1092:HIS:HE1	1:B:1196:ASP:H	1.41	0.68
1:A:88:THR:OG1	1:A:90:GLN:HG2	1.94	0.68
1:A:182:LYS:HB2	1:A:185:GLN:HG3	1.78	0.66
1:A:113:VAL:HG12	1:A:203:LEU:HD22	1.78	0.65
1:B:1071:CYS:HB2	1:B:1190:PHE:CE2	2.31	0.65
1:B:1097:ILE:CD1	1:B:1200:VAL:HG11	2.27	0.64
1:B:1182:LYS:HB2	1:B:1185:GLN:HG3	1.81	0.63
1:B:1151:TYR:O	1:B:1167:VAL:HG23	2.00	0.62
1:B:1097:ILE:HD13	1:B:1200:VAL:HG21	1.81	0.62
1:A:92:HIS:HE1	1:A:196:ASP:H	1.48	0.61
1:B:1122:ASN:HD21	1:B:1126:GLU:HG3	1.66	0.60
1:B:1195:VAL:O	1:B:1197:PRO:HD3	2.02	0.60
1:A:101:ILE:HD11	1:A:103:VAL:HG22	1.84	0.60
1:B:1122:ASN:ND2	1:B:1126:GLU:HG3	2.16	0.60
1:B:1160:ASP:OD2	1:B:1161:THR:HG23	2.03	0.59
1:A:160:ASP:OD2	1:A:161:THR:HG23	2.02	0.59
1:B:1080:LEU:HD11	1:B:1086:GLN:OE1	2.04	0.58
1:A:71:CYS:HB2	1:A:190:PHE:CE2	2.39	0.58
1:B:1146:ASN:O	1:B:1147:TRP:HB2	2.05	0.57
1:A:67:ARG:NE	1:B:1194:PRO:HB2	2.19	0.56
1:B:1097:ILE:CD1	1:B:1200:VAL:HG21	2.36	0.55
1:B:1168:ALA:O	1:B:1169:LEU:HD23	2.06	0.55
1:B:1069:LEU:HG	1:B:1190:PHE:HB3	1.89	0.55
1:B:1183:ARG:O	1:B:1189:HIS:HE1	1.90	0.55
1:A:200:VAL:N	1:A:201:PRO:HD3	2.22	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1200:VAL:N	1:B:1201:PRO:HD3	2.23	0.54
1:A:170:ASN:OD1	1:A:176:ARG:HD2	2.08	0.54
1:B:1119:LEU:HD12	1:B:1120:GLY:N	2.22	0.54
1:B:1145:GLU:O	1:B:1146:ASN:HB2	2.08	0.54
1:A:145:GLU:O	1:A:146:ASN:HB2	2.08	0.53
1:A:164:ARG:NE	3:A:2004:HOH:O	2.37	0.53
1:B:1065:ARG:NH1	1:B:1102:SER:HB2	2.23	0.52
1:A:146:ASN:O	1:A:147:TRP:HB2	2.10	0.52
1:A:168:ALA:HB2	1:A:188:THR:HG22	1.92	0.52
1:B:1097:ILE:HD12	1:B:1203:LEU:HD12	1.92	0.51
1:A:183:ARG:O	1:A:189:HIS:HE1	1.94	0.51
1:A:207:LEU:HD23	1:A:207:LEU:N	2.24	0.50
1:B:1113:VAL:CG1	1:B:1203:LEU:HD22	2.39	0.49
1:B:1053:GLY:O	1:B:1054:ALA:HB3	2.11	0.49
1:A:138:ILE:N	1:A:138:ILE:HD12	2.28	0.49
1:B:1091:ASP:OD2	1:B:1092:HIS:HD2	1.96	0.48
1:B:1092:HIS:CE1	1:B:1196:ASP:H	2.27	0.48
1:B:1122:ASN:OD1	1:B:1126:GLU:HG3	2.13	0.48
1:A:174:THR:HB	1:A:175:PRO:HD2	1.95	0.48
1:B:1174:THR:HB	1:B:1175:PRO:HD2	1.96	0.48
1:A:114:ASP:HB2	1:A:203:LEU:HD21	1.96	0.48
1:B:1170:ASN:ND2	1:B:1176:ARG:HH11	2.12	0.47
1:B:1088:THR:HG21	1:B:1093:SER:HB2	1.96	0.47
1:A:88:THR:HG21	1:A:93:SER:HB2	1.97	0.46
1:A:188:THR:HB	3:A:2003:HOH:O	2.15	0.46
1:B:1168:ALA:HB2	1:B:1188:THR:HG22	1.97	0.46
1:A:66:ARG:HA	1:A:99:GLU:HA	1.98	0.45
1:A:92:HIS:CE1	1:A:196:ASP:H	2.30	0.45
1:B:1065:ARG:HH12	1:B:1102:SER:HB2	1.81	0.45
1:B:1066:ARG:HA	1:B:1099:GLU:HA	1.99	0.45
1:A:81:PRO:HD3	1:A:95:PHE:CE2	2.52	0.45
1:B:1086:GLN:HE21	1:B:1086:GLN:HB3	1.57	0.45
1:B:1088:THR:OG1	1:B:1090:GLN:HB3	2.16	0.45
1:B:1141:GLU:HG3	1:B:1151:TYR:CE1	2.52	0.45
1:A:72:ARG:HG2	1:A:72:ARG:O	2.18	0.44
1:B:1122:ASN:CG	1:B:1126:GLU:HG3	2.38	0.44
1:B:1147:TRP:HA	1:B:1147:TRP:CE3	2.53	0.44
1:A:151:TYR:O	1:A:167:VAL:HG23	2.17	0.44
1:A:122:ASN:CG	1:A:126:GLU:HG3	2.36	0.44
1:A:90:GLN:HG3	1:A:93:SER:HB2	2.00	0.44
1:A:143:PHE:HE1	1:A:147:TRP:H	1.64	0.44
1:A:77:LEU:HD21	1:A:119:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1070:TYR:OH	1:B:1074:GLY:HA2	2.18	0.43
1:B:1119:LEU:HD12	1:B:1120:GLY:H	1.81	0.42
1:B:1068:GLN:HB2	1:B:1193:ARG:HB2	2.01	0.42
1:B:1111:ARG:HD3	1:B:1118:TYR:CE2	2.54	0.42
1:A:53:GLY:O	1:A:54:ALA:HB3	2.19	0.42
1:B:1062:GLY:O	1:B:1099:GLU:HG3	2.20	0.41
1:A:194:PRO:HB2	1:B:1067:ARG:CZ	2.50	0.41
1:A:88:THR:HG21	1:A:93:SER:CB	2.51	0.41
1:B:1193:ARG:HB3	1:B:1194:PRO:HD2	2.02	0.41
1:B:1188:THR:HB	3:B:2008:HOH:O	2.20	0.41
1:B:1207:LEU:H	1:B:1207:LEU:HG	1.70	0.41
1:B:1124:LYS:HB2	1:B:1124:LYS:HE3	1.89	0.41
1:B:1121:MET:O	1:B:1136:GLU:HB3	2.21	0.40
1:A:101:ILE:HG12	1:A:109:SER:HB2	2.02	0.40
1:A:122:ASN:OD1	1:A:126:GLU:HG3	2.21	0.40
1:A:176:ARG:HH11	1:A:176:ARG:HG3	1.86	0.40
1:B:1176:ARG:HG3	1:B:1176:ARG:HH11	1.85	0.40
1:A:68:GLN:HB2	1:A:193:ARG:HB2	2.04	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	155/211 (74%)	145 (94%)	8 (5%)	2 (1%)	18	29
1	B	155/211 (74%)	144 (93%)	9 (6%)	2 (1%)	18	29
All	All	310/422 (74%)	289 (93%)	17 (6%)	4 (1%)	18	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	B	1145	GLU

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Mol	Chain	Res	Type
1	A	54	ALA
1	B	1054	ALA

### 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	132/172 (77%)	123 (93%)	9 (7%)	22	39
1	B	131/172 (76%)	127 (97%)	4 (3%)	52	79
All	All	263/344 (76%)	250 (95%)	13 (5%)	35	59

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	65	ARG
1	A	101	ILE
1	A	109	SER
1	A	111	ARG
1	A	142	GLN
1	A	150	THR
1	A	189	HIS
1	A	207	LEU
1	B	1086	GLN
1	B	1126	GLU
1	B	1198	GLU
1	B	1207	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	92	HIS
1	A	146	ASN
1	A	189	HIS
1	B	1092	HIS

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Mol	Chain	Res	Type
1	B	1146	ASN
1	B	1189	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	0.32	0	6,6,6	0.13	0
2	SO4	A	302	-	4,4,4	0.35	0	6,6,6	0.10	0
2	SO4	A	303	-	4,4,4	0.49	0	6,6,6	0.15	0
2	SO4	B	300	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	B	304	-	4,4,4	0.51	0	6,6,6	0.15	0
2	SO4	B	305	-	4,4,4	0.40	0	6,6,6	0.19	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
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	303	-	-	0/0/0/0	0/0/0/0
2	SO4	B	300	-	-	0/0/0/0	0/0/0/0
2	SO4	B	304	-	-	0/0/0/0	0/0/0/0
2	SO4	B	305	-	-	0/0/0/0	0/0/0/0

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	157/211 (74%)	2.26	90 (57%) <b>0</b> <b>0</b>	58, 71, 88, 113	0
1	B	157/211 (74%)	2.27	87 (55%) <b>0</b> <b>0</b>	58, 71, 88, 114	0
All	All	314/422 (74%)	2.27	177 (56%) <b>0</b> <b>0</b>	58, 71, 88, 114	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	7.3
1	A	75	PHE	6.2
1	B	1208	LEU	5.8
1	A	204	TYR	5.4
1	B	1139	PHE	5.1
1	B	1075	PHE	5.0
1	B	1138	ILE	4.9
1	B	1079	ILE	4.8
1	B	1204	TYR	4.8
1	B	1169	LEU	4.5
1	A	79	ILE	4.3
1	A	61	HIS	4.3
1	A	139	PHE	4.2
1	A	138	ILE	4.2
1	A	106	GLY	4.1
1	A	169	LEU	4.0
1	B	1191	LEU	4.0
1	B	1203	LEU	4.0
1	A	118	TYR	3.9
1	B	1057	LEU	3.9
1	B	1077	LEU	3.9
1	A	96	GLY	3.8
1	B	1096	GLY	3.8
1	A	203	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	1063	ILE	3.8
1	B	1118	TYR	3.8
1	A	178	GLY	3.8
1	B	1155	ILE	3.8
1	A	129	GLY	3.7
1	B	1128	TYR	3.7
1	A	187	PHE	3.7
1	A	197	PRO	3.7
1	B	1103	VAL	3.7
1	A	110	ILE	3.7
1	B	1168	ALA	3.7
1	A	74	GLY	3.7
1	B	1129	GLY	3.6
1	A	127	LEU	3.5
1	B	1117	LEU	3.5
1	A	128	TYR	3.5
1	B	1061	HIS	3.5
1	B	1071	CYS	3.5
1	A	57	LEU	3.4
1	A	63	ILE	3.4
1	A	168	ALA	3.4
1	A	98	LEU	3.4
1	A	77	LEU	3.4
1	A	71	CYS	3.3
1	A	103	VAL	3.3
1	B	1207	LEU	3.3
1	B	1070	TYR	3.3
1	A	190	PHE	3.2
1	B	1076	HIS	3.2
1	A	100	PHE	3.2
1	B	1100	PHE	3.2
1	A	76	HIS	3.2
1	B	1098	LEU	3.2
1	B	1110	ILE	3.1
1	B	1106	GLY	3.1
1	A	148	TYR	3.1
1	A	95	PHE	3.1
1	B	1088	THR	3.1
1	B	1116	GLY	3.1
1	B	1127	LEU	3.1
1	A	58	ALA	3.1
1	B	1187	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	191	LEU	3.1
1	B	1095	PHE	3.1
1	B	1142	GLN	3.1
1	B	1178	GLY	3.1
1	A	165	TYR	3.0
1	A	155	ILE	3.0
1	A	87	GLY	3.0
1	A	119	LEU	3.0
1	B	1194	PRO	3.0
1	A	180	ARG	3.0
1	B	1087	GLY	3.0
1	B	1150	THR	2.9
1	A	195	VAL	2.9
1	B	1161	THR	2.9
1	A	104	ALA	2.9
1	B	1072	ARG	2.9
1	B	1190	PHE	2.8
1	A	122	ASN	2.8
1	A	194	PRO	2.8
1	A	152	SER	2.8
1	B	1152	SER	2.8
1	B	1080	LEU	2.8
1	A	192	PRO	2.8
1	B	1197	PRO	2.8
1	A	117	LEU	2.8
1	A	72	ARG	2.7
1	A	88	THR	2.7
1	B	1192	PRO	2.7
1	A	170	ASN	2.7
1	A	70	TYR	2.7
1	A	150	THR	2.7
1	B	1104	ALA	2.7
1	A	154	ASN	2.7
1	B	1137	CYS	2.6
1	B	1170	ASN	2.6
1	B	1058	ALA	2.6
1	A	80	LEU	2.6
1	A	130	SER	2.6
1	B	1167	VAL	2.6
1	A	161	THR	2.6
1	B	1173	GLY	2.6
1	A	151	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	173	GLY	2.5
1	A	67	ARG	2.5
1	A	60	LEU	2.5
1	B	1105	VAL	2.5
1	B	1195	VAL	2.5
1	B	1166	PHE	2.5
1	B	1122	ASN	2.5
1	A	156	TYR	2.5
1	B	1130	SER	2.5
1	B	1165	TYR	2.4
1	B	1200	VAL	2.4
1	A	188	THR	2.4
1	B	1149	ASN	2.4
1	B	1125	GLY	2.4
1	B	1066	ARG	2.4
1	B	1148	TYR	2.4
1	B	1097	ILE	2.4
1	B	1154	ASN	2.4
1	A	94	LEU	2.4
1	A	167	VAL	2.4
1	A	189	HIS	2.4
1	B	1151	TYR	2.4
1	B	1180	ARG	2.3
1	A	137	CYS	2.3
1	A	97	ILE	2.3
1	A	200	VAL	2.3
1	B	1121	MET	2.3
1	A	142	GLN	2.3
1	A	131	GLU	2.3
1	B	1055	ALA	2.3
1	A	105	VAL	2.3
1	B	1108	VAL	2.3
1	A	83	GLY	2.3
1	A	55	ALA	2.3
1	A	132	LYS	2.3
1	A	102	SER	2.3
1	B	1188	THR	2.3
1	B	1156	TYR	2.2
1	B	1083	GLY	2.2
1	A	166	PHE	2.2
1	B	1199	ARG	2.2
1	A	196	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	176	ARG	2.2
1	B	1067	ARG	2.2
1	B	1102	SER	2.2
1	A	116	GLY	2.2
1	A	171	LYS	2.2
1	B	1133	LEU	2.1
1	A	121	MET	2.1
1	B	1196	ASP	2.1
1	A	125	GLY	2.1
1	B	1135	SER	2.1
1	B	1113	VAL	2.1
1	A	81	PRO	2.1
1	B	1123	ASP	2.1
1	B	1059	HIS	2.1
1	A	84	SER	2.1
1	B	1084	SER	2.1
1	B	1143	PHE	2.1
1	A	66	ARG	2.1
1	A	115	SER	2.1
1	A	147	TRP	2.1
1	A	149	ASN	2.1
1	B	1176	ARG	2.0
1	B	1189	HIS	2.0
1	A	89	ARG	2.0
1	A	65	ARG	2.0
1	B	1081	PRO	2.0
1	A	143	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	304	5/5	0.33	0.57	119,120,120,120	0
2	SO4	A	303	5/5	0.25	-1.04	120,120,120,120	0
2	SO4	B	300	5/5	0.24	-1.08	118,119,119,120	0
2	SO4	A	302	5/5	0.21	-1.20	118,119,119,120	0
2	SO4	B	305	5/5	0.21	-3.71	118,120,120,120	0
2	SO4	A	301	5/5	0.19	-4.00	117,117,118,118	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.