



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:34 PM GMT

PDB ID : 3C7Q  
Title : Structure of VEGFR2 kinase domain in complex with BIBF1120  
Authors : Hilberg, F.; Roth, G.J.; Krssak, M.; Kautschitsch, S.; Sommergruber, W.;  
Tontsch-Grunt, U.; Garin-Chesa, P.; Bader, G.; Zoephel, A.; Quant, J.; Heckel,  
A.; Rettig, W.J.  
Deposited on : 2008-02-08  
Resolution : 2.10 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>

---

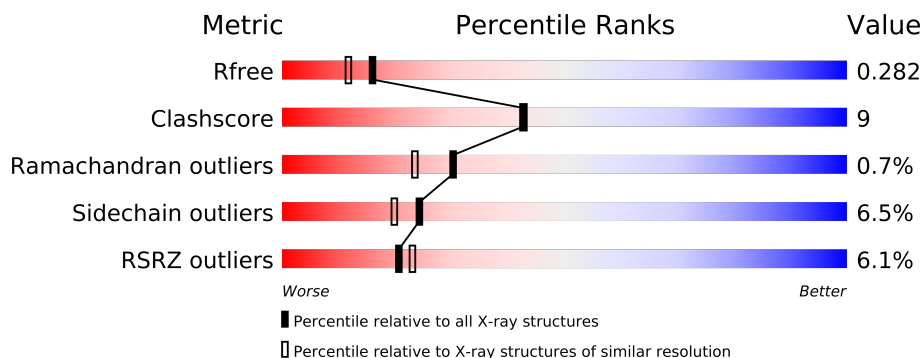
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	316	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	3	-	X
2	SO4	A	6	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2633 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 Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	291	2362	1508	407	426	2	19	27	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	804	GLY	-	EXPRESSION TAG	UNP P35968
A	805	SER	-	EXPRESSION TAG	UNP P35968
A	?	-	THR	DELETION	UNP P35968
A	?	-	LYS	DELETION	UNP P35968
A	?	-	GLY	DELETION	UNP P35968
A	?	-	ALA	DELETION	UNP P35968
A	?	-	ARG	DELETION	UNP P35968
A	?	-	PHE	DELETION	UNP P35968
A	?	-	ARG	DELETION	UNP P35968
A	?	-	GLN	DELETION	UNP P35968
A	?	-	GLY	DELETION	UNP P35968
A	?	-	LYS	DELETION	UNP P35968
A	?	-	ASP	DELETION	UNP P35968
A	?	-	TYR	DELETION	UNP P35968
A	?	-	VAL	DELETION	UNP P35968
A	?	-	GLY	DELETION	UNP P35968
A	?	-	ALA	DELETION	UNP P35968
A	?	-	ILE	DELETION	UNP P35968
A	?	-	PRO	DELETION	UNP P35968
A	?	-	VAL	DELETION	UNP P35968
A	?	-	ASP	DELETION	UNP P35968
A	?	-	LEU	DELETION	UNP P35968
A	?	-	LYS	DELETION	UNP P35968
A	?	-	ARG	DELETION	UNP P35968
A	?	-	ARG	DELETION	UNP P35968
A	?	-	LEU	DELETION	UNP P35968
A	?	-	ASP	DELETION	UNP P35968

*Continued on next page...*

*Continued from previous page...*

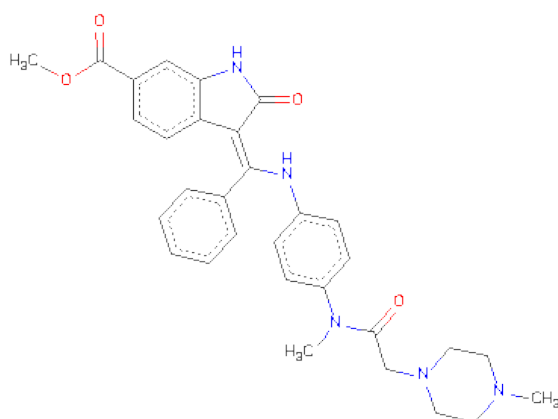
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP P35968
A	?	-	ILE	DELETION	UNP P35968
A	?	-	THR	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	GLN	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	ALA	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	GLY	DELETION	UNP P35968
A	?	-	PHE	DELETION	UNP P35968
A	?	-	VAL	DELETION	UNP P35968
A	?	-	GLU	DELETION	UNP P35968
A	?	-	GLU	DELETION	UNP P35968
A	?	-	LYS	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	LEU	DELETION	UNP P35968
A	?	-	SER	DELETION	UNP P35968
A	?	-	ASP	DELETION	UNP P35968
A	?	-	VAL	DELETION	UNP P35968
A	?	-	GLU	DELETION	UNP P35968
A	?	-	GLU	DELETION	UNP P35968
A	?	-	GLU	DELETION	UNP P35968
A	?	-	GLU	DELETION	UNP P35968
A	?	-	ALA	DELETION	UNP P35968

- Molecule 2 is SULFATE ION (three-letter code: SO4) (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	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is METHYL (3Z)-3-[[[4-{METHYL[(4-METHYLPIPERAZIN-1-YL)ACETYL]AMINO}PHENYL)AMINO](PHENYL)METHYLIDENE}-2-OXO-2,3-DIHYDRO-1H-INDOLE-6-CARBOXYLATE (three-letter code: XIN) (formula: C<sub>31</sub>H<sub>33</sub>N<sub>5</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			40	31	5	4		

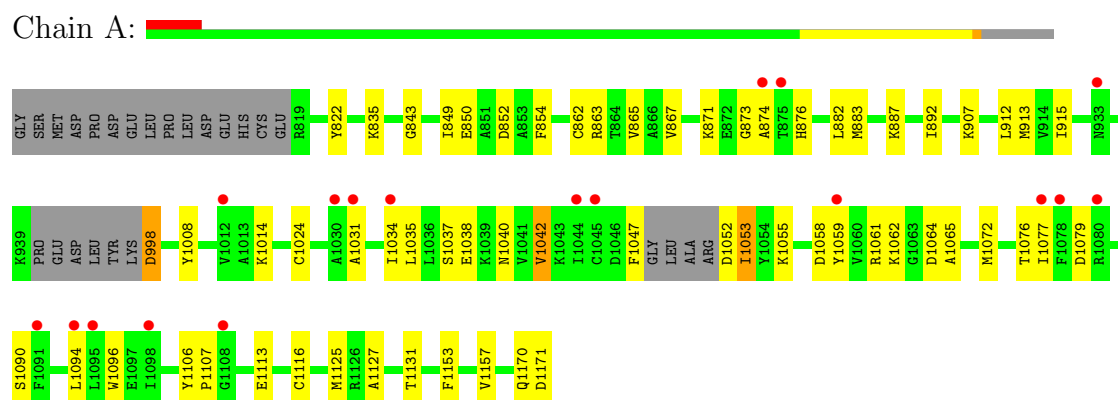
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		

### 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 ( $\text{RSRZ} > 2$ ). 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: Vascular endothelial growth factor receptor 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.25Å 94.44Å 96.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.54 – 2.10 28.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.54-2.10) 99.6 (28.54-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.217 , 0.279 0.218 , 0.282	Depositor DCC
$R_{free}$ test set	1050 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.6	EDS
Estimated twinning fraction	0.027 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 20985 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: CME, SO4, XIN, PTR

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	0.71	1/2349 (0.0%)	0.76	1/3162 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	907	LYS	CE-NZ	-7.07	1.31	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1058	ASP	CB-CG-OD1	6.11	123.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	ILE	Peptide

## 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	2362	0	2349	42	0
2	A	25	0	0	0	1
3	A	40	0	33	0	0
4	A	206	0	0	5	1
All	All	2633	0	2382	42	1

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 9.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1096:TRP:CE2	1:A:1125:MET:HE2	1.87	1.08
1:A:1096:TRP:CE2	1:A:1125:MET:CE	2.47	0.97
1:A:1072:MET:HE3	1:A:1076:THR:HG22	1.64	0.77
1:A:1096:TRP:NE1	1:A:1125:MET:HE2	2.02	0.74
1:A:1096:TRP:CZ2	1:A:1125:MET:CE	2.73	0.71
1:A:1096:TRP:CD2	1:A:1125:MET:HE1	2.29	0.68
1:A:1096:TRP:CE2	1:A:1125:MET:HE1	2.31	0.65
1:A:1096:TRP:CD2	1:A:1125:MET:CE	2.81	0.63
1:A:1064:ASP:O	4:A:1376:HOH:O	2.16	0.63
1:A:1072:MET:CE	1:A:1076:THR:HG22	2.27	0.63
1:A:1034:ILE:HG22	1:A:1042:VAL:HG22	1.85	0.57
1:A:849:ILE:HG22	1:A:850:GLU:O	2.04	0.57
1:A:854:PHE:HB2	1:A:862:CME:HE2	1.88	0.55
1:A:1171:ASP:C	1:A:1171:ASP:OD1	2.45	0.55
1:A:865:VAL:HG21	1:A:915:ILE:CG2	2.39	0.52
1:A:1153:PHE:O	1:A:1157:VAL:HG23	2.11	0.51
1:A:1031:ALA:HB2	1:A:1094:LEU:CD1	2.41	0.50
1:A:1052:ASP:HB3	4:A:1340:HOH:O	2.11	0.49
1:A:1059:PTR:O2P	1:A:1059:PTR:HE2	2.12	0.48
1:A:822:TYR:HB2	1:A:887:LYS:HE2	1.94	0.48
1:A:1096:TRP:CE3	1:A:1125:MET:HE1	2.49	0.48
1:A:1065:ALA:HA	4:A:1376:HOH:O	2.14	0.47
1:A:876:HIS:NE2	4:A:1274:HOH:O	2.34	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:883:MET:O	1:A:887:LYS:HG2	2.15	0.46
1:A:892:ILE:HD11	1:A:1024:CME:SD	2.55	0.46
1:A:1072:MET:HB3	1:A:1072:MET:HE2	1.77	0.45
1:A:1008:TYR:OH	1:A:1040:ASN:ND2	2.50	0.44
1:A:865:VAL:HG21	1:A:915:ILE:HG23	1.98	0.44
1:A:892:ILE:N	1:A:892:ILE:HD13	2.32	0.43
1:A:892:ILE:HD12	1:A:1024:CME:SG	2.58	0.43
1:A:1077:ILE:HG21	1:A:1116:CYS:SG	2.59	0.43
1:A:1107:PRO:HD3	1:A:1125:MET:HE3	2.01	0.42
1:A:1038:GLU:HG2	1:A:1038:GLU:H	1.62	0.42
1:A:854:PHE:HB2	1:A:862:CME:CE	2.48	0.42
1:A:867:VAL:CG1	1:A:913:MET:HB3	2.49	0.42
1:A:998:ASP:HA	4:A:1346:HOH:O	2.20	0.41
1:A:1127:ALA:HB1	1:A:1131:THR:HG21	2.03	0.41
1:A:1096:TRP:CZ2	1:A:1125:MET:HE2	2.41	0.41
1:A:843:GLY:O	1:A:871:LYS:NZ	2.46	0.41
1:A:1106:TYR:CE1	1:A:1125:MET:HG3	2.57	0.40
1:A:871:LYS:O	1:A:874:ALA:HB2	2.22	0.40
1:A:882:LEU:HD23	1:A:912:LEU:HD23	2.04	0.40

All (1) 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	Distance(Å)	Clash(Å)
2:A:1:SO4:O1	4:A:1275:HOH:O[1_455]	2.05	0.15

## 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	280/316 (89%)	265 (95%)	13 (5%)	2 (1%)	30	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1053	ILE
1	A	873	GLY

### 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	248/270 (92%)	232 (94%)	16 (6%)	24	20

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	835	LYS
1	A	852	ASP
1	A	863	ARG
1	A	998	ASP
1	A	1014	LYS
1	A	1035	LEU
1	A	1037	SER
1	A	1042	VAL
1	A	1047	PHE
1	A	1055	LYS
1	A	1061	ARG
1	A	1062	LYS
1	A	1079	ASP
1	A	1090	SER
1	A	1113	GLU
1	A	1170	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1040	ASN
1	A	1085	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CME	A	1007	1	9,9,10	5.58	1 (11%)	7,9,11	1.28	1 (14%)
1	CME	A	1024	1	9,9,10	5.77	1 (11%)	7,9,11	1.25	1 (14%)
1	PTR	A	1054	1	16,16,17	4.99	3 (18%)	20,22,24	5.55	2 (10%)
1	PTR	A	1059	1	16,16,17	3.62	3 (18%)	20,22,24	0.86	0
1	CME	A	862	1	9,9,10	6.32	2 (22%)	7,9,11	1.91	2 (28%)

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
1	CME	A	1007	1	-	0/6/8/10	0/0/0/0
1	CME	A	1024	1	-	0/6/8/10	0/0/0/0
1	PTR	A	1054	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1059	1	-	0/9/11/13	0/1/1/1
1	CME	A	862	1	-	0/6/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	862	CME	O-C	18.71	1.24	1.11
1	A	1054	PTR	O-C	18.33	1.24	1.11
1	A	1024	CME	O-C	17.13	1.23	1.11
1	A	1007	CME	O-C	16.56	1.22	1.11

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1059	PTR	O-C	12.59	1.20	1.11
1	A	1054	PTR	OH-CZ	-6.96	1.22	1.40
1	A	1059	PTR	OH-CZ	-6.42	1.24	1.40
1	A	1054	PTR	CA-C	3.36	1.54	1.48
1	A	1059	PTR	P-O1P	-2.34	1.43	1.51
1	A	862	CME	CB-SG	-2.31	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1054	PTR	C-CA-N	24.59	138.39	113.83
1	A	862	CME	CB-SG-SD	4.18	112.21	103.87
1	A	1007	CME	CB-SG-SD	3.21	110.27	103.87
1	A	862	CME	CE-SD-SG	-2.52	90.49	103.50
1	A	1024	CME	CB-SG-SD	2.30	108.45	103.87
1	A	1054	PTR	CG-CB-CA	-2.22	109.19	114.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	1	-	4,4,4	0.18	0	6,6,6	0.13	0
3	XIN	A	1172	-	44,44,44	1.37	7 (15%)	62,62,62	1.73	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	2	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	A	3	-	4,4,4	0.15	0	6,6,6	0.40	0
2	SO4	A	4	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	A	6	-	4,4,4	0.13	0	6,6,6	0.07	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	1	-	-	0/0/0/0	0/0/0/0
3	XIN	A	1172	-	-	0/30/52/52	0/3/5/5
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	A	4	-	-	0/0/0/0	0/0/0/0
2	SO4	A	6	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1172	XIN	O10-C4	-4.19	1.15	1.23
3	A	1172	XIN	C15-N8	-3.17	1.35	1.41
3	A	1172	XIN	C19-C15	-3.06	1.34	1.39
3	A	1172	XIN	C1-C3	-2.28	1.34	1.40
3	A	1172	XIN	O25-C28	-2.28	1.39	1.45
3	A	1172	XIN	C2-C5	-2.18	1.38	1.41
3	A	1172	XIN	C6-C2	-2.06	1.36	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1172	XIN	C1-C3-N8	6.37	123.29	118.09
3	A	1172	XIN	C24-C27-N29	4.75	126.09	120.11
3	A	1172	XIN	C20-C15-N8	3.62	132.55	120.39
3	A	1172	XIN	C32-N34-C36	3.22	115.64	110.99
3	A	1172	XIN	C15-N8-C3	2.97	137.86	127.87
3	A	1172	XIN	C19-C15-N8	-2.78	111.06	120.39
3	A	1172	XIN	C36-C38-N39	2.50	113.58	110.82
3	A	1172	XIN	C24-C20-C15	2.29	122.94	120.27
3	A	1172	XIN	C7-C3-C1	-2.29	120.00	122.42
3	A	1172	XIN	C38-N39-C37	2.21	112.62	109.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1172	XIN	C19-C23-C27	2.13	123.30	120.44
3	A	1172	XIN	C28-O25-C21	-2.10	111.27	115.87

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	291/316 (92%)	0.38	18 (6%)	20 22	14, 28, 46, 52	7 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	874	ALA	4.3
1	A	1108	GLY	3.9
1	A	1059	PTR	2.9
1	A	1078	PHE	2.9
1	A	1095	LEU	2.7
1	A	1098	ILE	2.7
1	A	875	THR	2.6
1	A	1080	ARG	2.5
1	A	933	ASN	2.4
1	A	1030	ALA	2.4
1	A	1034	ILE	2.4
1	A	1031	ALA	2.3
1	A	1012	VAL	2.3
1	A	1077	ILE	2.3
1	A	1094	LEU	2.2
1	A	1091	PHE	2.1
1	A	1045	CYS	2.0
1	A	1044	ILE	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
1	PTR	A	1059	16/17	0.30	2.21	41,46,55,56	0
1	CME	A	862	10/11	0.18	1.33	32,35,47,49	0
1	CME	A	1024	10/11	0.18	0.96	34,36,51,53	0
1	PTR	A	1054	16/17	0.19	-0.24	41,42,43,44	0
1	CME	A	1007	10/11	0.13	-1.00	19,21,27,28	0

### 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	3	5/5	0.25	3.81	73,74,74,75	0
2	SO4	A	6	5/5	0.30	3.25	80,80,80,80	0
2	SO4	A	4	5/5	0.20	1.32	72,72,72,72	0
2	SO4	A	1	5/5	0.20	1.25	65,66,68,68	0
3	XIN	A	1172	40/40	0.13	0.21	20,25,43,45	0
2	SO4	A	2	5/5	0.15	-4.19	90,90,91,91	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.