



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:35 PM GMT

PDB ID : 3O2X  
Title : MMP-13 in complex with selective tetrazole core inhibitor  
Authors : Kiefer, J.R.; Barta, T.E.; Becker, D.P.; Mathis, K.J.; Williams, J.  
Deposited on : 2010-07-22  
Resolution : 1.90 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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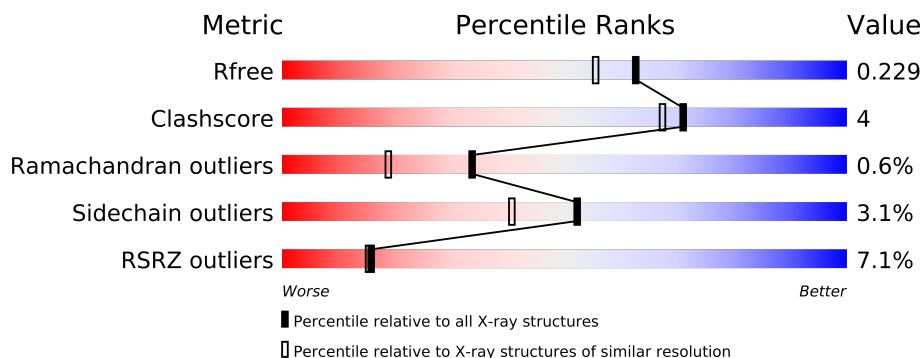
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	164	
1	B	164	
1	C	164	
1	D	164	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	B	3	-	X
6	EPE	A	400	-	X
6	EPE	B	400	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6167 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.

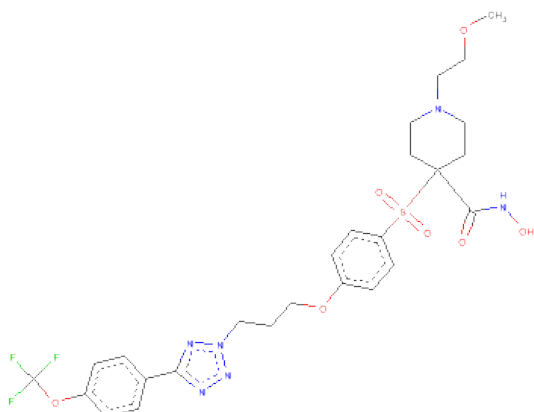
- Molecule 1 is a protein called Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	2	0
			1314	848	213	248	5			
1	B	164	Total	C	N	O	S	0	0	0
			1300	841	211	243	5			
1	C	164	Total	C	N	O	S	0	2	0
			1314	850	213	246	5			
1	D	164	Total	C	N	O	S	0	0	0
			1300	841	211	243	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1104	ALA	-	expression tag	UNP P45452
B	2104	ALA	-	expression tag	UNP P45452
C	1104	ALA	-	expression tag	UNP P45452
D	2104	ALA	-	expression tag	UNP P45452

- Molecule 2 is N-HYDROXY-1-(2-METHOXYETHYL)-4-{{[4-(3-{5-[4-(TRIFLUOROMETHOXY)PHENYL]-2H-TETRAZOL-2-YL}PROPOXY)PHENYL]SULFONYL}PIPERIDINE-4-CARBOXAMIDE (three-letter code: 3O2) (formula: C<sub>26</sub>H<sub>31</sub>F<sub>3</sub>N<sub>6</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 43	C 26	F 3	N 6	O 7	S 1	0	0
2	B	1	Total 43	C 26	F 3	N 6	O 7	S 1	0	0
2	C	1	Total 43	C 26	F 3	N 6	O 7	S 1	0	0
2	D	1	Total 43	C 26	F 3	N 6	O 7	S 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

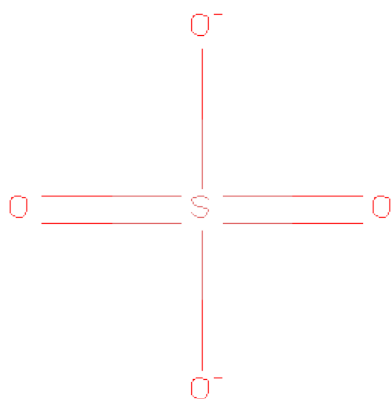
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	D	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



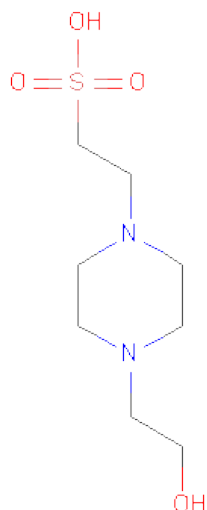
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

- Molecule 7 is water.

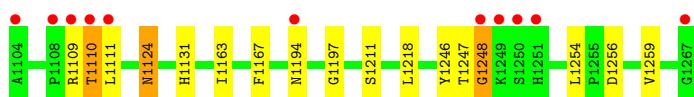
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	173	Total	O	0	0
			173	173		
7	B	151	Total	O	0	0
			151	151		
7	C	180	Total	O	0	0
			180	180		
7	D	178	Total	O	0	0
			178	178		

### 3 Residue-property plots i

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.

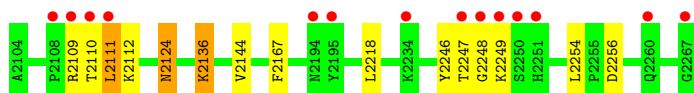
#### • Molecule 1: Collagenase 3

Chain A: 



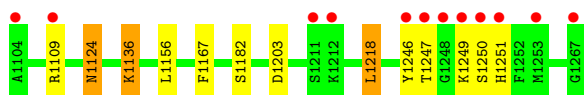
#### • Molecule 1: Collagenase 3

Chain B: 



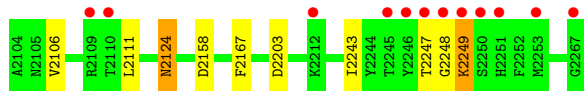
#### • Molecule 1: Collagenase 3

Chain C: 



#### • Molecule 1: Collagenase 3

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.86Å 95.26Å 120.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 1.90 19.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.1 (19.72-1.90) 84.1 (19.72-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.31 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.177 , 0.210 0.194 , 0.229	Depositor DCC
$R_{free}$ test set	2879 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 26.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 56646 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8373e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: EPE, ZN, 3O2, CA, 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	0.33	0/1360	0.49	0/1848
1	B	0.35	0/1346	0.52	0/1829
1	C	0.34	0/1360	0.50	0/1848
1	D	0.33	0/1346	0.49	0/1829
All	All	0.34	0/5412	0.50	0/7354

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2247	THR	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	1314	0	1218	11	0
1	B	1300	0	1211	15	0
1	C	1314	0	1225	14	0
1	D	1300	0	1211	8	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	1	0
2	D	43	0	30	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	15	0	0	0	0
5	B	15	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	173	0	0	0	0
7	B	151	0	0	1	0
7	C	180	0	0	1	0
7	D	178	0	0	2	0
All	All	6167	0	5009	47	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 4.

All (47) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:2124:ASN:HD21	1:D:2167:PHE:H	1.07	0.95
1:C:1124:ASN:HD21	1:C:1167:PHE:H	1.06	0.95
1:A:1218:LEU:HD22	1:A:1246:TYR:HB2	1.56	0.88
1:B:2109:ARG:HB3	1:B:2110:THR:HA	1.63	0.81
1:B:2109:ARG:CB	1:B:2110:THR:HA	2.15	0.75
1:D:2111:LEU:HD23	7:D:860:HOH:O	1.92	0.69
1:C:1156:LEU:HD13	1:D:2243:ILE:HD13	1.77	0.66
1:C:1250:SER:CB	1:C:1251:HIS:HA	2.26	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2124:ASN:HD21	1:B:2167:PHE:H	1.44	0.63
1:C:1218[B]:LEU:HD12	1:C:1246:TYR:HB2	1.82	0.62
1:B:2124:ASN:ND2	1:B:2167:PHE:H	1.99	0.60
1:D:2124:ASN:ND2	1:D:2167:PHE:H	1.88	0.59
1:A:1218:LEU:CD2	1:A:1246:TYR:HB2	2.29	0.59
1:B:2111:LEU:HD22	1:B:2112:LYS:HG2	1.85	0.59
1:B:2136:LYS:N	1:B:2136:LYS:HD3	2.17	0.59
1:C:1218[A]:LEU:HD21	2:C:1801:3O2:H17	1.86	0.56
1:A:1124:ASN:HD21	1:A:1167:PHE:H	1.54	0.55
1:D:2248:GLY:O	1:D:2249:LYS:CB	2.55	0.54
1:C:1250:SER:CB	1:C:1251:HIS:CA	2.86	0.53
1:A:1124:ASN:ND2	1:A:1167:PHE:H	2.07	0.52
1:C:1124:ASN:ND2	1:C:1167:PHE:H	1.90	0.52
1:C:1250:SER:HB2	1:C:1251:HIS:HA	1.90	0.51
1:D:2124:ASN:HD21	1:D:2167:PHE:N	1.91	0.51
1:C:1250:SER:HB3	1:C:1251:HIS:C	2.32	0.50
1:B:2246:TYR:HB3	1:B:2247:THR:HA	1.94	0.50
1:D:2106:VAL:HG22	7:D:794:HOH:O	2.12	0.49
1:D:2124:ASN:HD22	1:D:2124:ASN:C	2.16	0.48
1:C:1250:SER:HB3	1:C:1251:HIS:HA	1.97	0.47
1:C:1136:LYS:HD3	1:C:1136:LYS:N	2.29	0.47
1:C:1247:THR:HG23	1:C:1249:LYS:H	1.78	0.47
1:A:1247:THR:HG22	7:B:320:HOH:O	2.15	0.47
1:A:1109:ARG:HB3	1:A:1110:THR:CA	2.45	0.46
1:B:2218:LEU:HD13	1:B:2246:TYR:O	2.15	0.46
1:A:1218:LEU:HD22	1:A:1246:TYR:CB	2.38	0.45
1:C:1250:SER:HB3	1:C:1251:HIS:CA	2.46	0.45
1:B:2247:THR:N	1:B:2248:GLY:HA2	2.32	0.45
1:A:1211:SER:HB3	1:A:1248:GLY:HA2	1.99	0.45
1:B:2218:LEU:CD1	1:B:2246:TYR:O	2.65	0.45
1:B:2111:LEU:HD22	1:B:2112:LYS:CG	2.46	0.44
1:B:2144:VAL:CG1	1:B:2254:LEU:HD13	2.48	0.44
1:A:1109:ARG:HB3	1:A:1110:THR:CB	2.49	0.43
1:C:1247:THR:HG22	7:C:392:HOH:O	2.18	0.42
1:B:2110:THR:OG1	1:B:2111:LEU:N	2.52	0.42
1:A:1254:LEU:HD23	1:A:1259:VAL:HG22	2.01	0.42
1:A:1163:ILE:HG23	1:A:1197:GLY:O	2.19	0.42
1:B:2247:THR:N	1:B:2248:GLY:CA	2.83	0.41
1:B:2248:GLY:N	1:B:2249:LYS:HA	2.37	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	164/164 (100%)	155 (94%)	7 (4%)	2 (1%)	19	6
1	B	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	C	164/164 (100%)	156 (95%)	7 (4%)	1 (1%)	33	19
1	D	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	33	19
All	All	652/656 (99%)	617 (95%)	31 (5%)	4 (1%)	33	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2249	LYS
1	A	1194	ASN
1	A	1248	GLY
1	C	1109	ARG

### 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	140/139 (101%)	134 (96%)	6 (4%)	40	26
1	B	138/139 (99%)	134 (97%)	4 (3%)	55	44
1	C	140/139 (101%)	134 (96%)	6 (4%)	40	26
1	D	138/139 (99%)	135 (98%)	3 (2%)	64	57
All	All	556/556 (100%)	537 (97%)	19 (3%)	52	36

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1110	THR
1	A	1111	LEU
1	A	1124	ASN
1	A	1131	HIS
1	A	1256[A]	ASP
1	A	1256[B]	ASP
1	B	2111	LEU
1	B	2124	ASN
1	B	2136	LYS
1	B	2256	ASP
1	C	1124	ASN
1	C	1136	LYS
1	C	1182	SER
1	C	1203	ASP
1	C	1218[A]	LEU
1	C	1218[B]	LEU
1	D	2124	ASN
1	D	2158	ASP
1	D	2203	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1124	ASN
1	A	1131	HIS
1	B	2124	ASN
1	C	1124	ASN
1	C	1131	HIS
1	D	2124	ASN

### 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 ⓘ

Of 31 ligands modelled in this entry, 16 are monoatomic - leaving 15 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$
2	3O2	A	1801	3	46,46,46	1.09	2 (4%)	66,66,66	1.87	12 (18%)
5	SO4	A	2	-	4,4,4	0.23	0	6,6,6	0.09	0
6	EPE	A	400	-	12,12,15	0.92	1 (8%)	16,16,20	3.91	3 (18%)
5	SO4	A	7	-	4,4,4	0.18	0	6,6,6	0.07	0
5	SO4	A	9	-	4,4,4	0.22	0	6,6,6	0.07	0
2	3O2	B	1801	3	46,46,46	1.08	2 (4%)	66,66,66	1.90	13 (19%)
5	SO4	B	3	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	B	4	-	4,4,4	0.26	0	6,6,6	0.13	0
6	EPE	B	400	-	12,12,15	0.95	1 (8%)	16,16,20	3.88	4 (25%)
5	SO4	B	6	-	4,4,4	0.18	0	6,6,6	0.12	0
5	SO4	C	1	-	4,4,4	0.25	0	6,6,6	0.14	0
2	3O2	C	1801	3	46,46,46	1.07	1 (2%)	66,66,66	1.95	11 (16%)
2	3O2	D	1801	3	46,46,46	1.07	3 (6%)	66,66,66	1.78	11 (16%)
5	SO4	D	5	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	D	8	-	4,4,4	0.15	0	6,6,6	0.08	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	3O2	A	1801	3	-	0/41/55/55	0/4/4/4
5	SO4	A	2	-	-	0/0/0/0	0/0/0/0
6	EPE	A	400	-	-	0/6/14/19	0/1/1/1
5	SO4	A	7	-	-	0/0/0/0	0/0/0/0
5	SO4	A	9	-	-	0/0/0/0	0/0/0/0
2	3O2	B	1801	3	-	0/41/55/55	0/4/4/4
5	SO4	B	3	-	-	0/0/0/0	0/0/0/0
5	SO4	B	4	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	B	400	-	-	0/6/14/19	0/1/1/1
5	SO4	B	6	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1	-	-	0/0/0/0	0/0/0/0
2	3O2	C	1801	3	-	0/41/55/55	0/4/4/4
2	3O2	D	1801	3	-	0/41/55/55	0/4/4/4
5	SO4	D	5	-	-	0/0/0/0	0/0/0/0
5	SO4	D	8	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1801	3O2	C19-N5	4.41	1.37	1.34
2	A	1801	3O2	C19-N5	4.35	1.37	1.34
2	C	1801	3O2	C19-N5	4.35	1.37	1.34
2	D	1801	3O2	C19-N5	4.08	1.37	1.34
6	B	400	EPE	C10-S	2.68	1.81	1.77
6	A	400	EPE	C10-S	2.67	1.81	1.77
2	D	1801	3O2	C6-N2	2.15	1.38	1.34
2	A	1801	3O2	C1-S1	-2.12	1.80	1.83
2	D	1801	3O2	C1-S1	-2.06	1.80	1.83
2	B	1801	3O2	C6-N2	2.01	1.37	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	400	EPE	C5-N4-C3	14.16	119.32	110.50
6	B	400	EPE	C5-N4-C3	14.06	119.26	110.50
2	C	1801	3O2	O6-N2-C6	-7.49	109.74	119.80
2	B	1801	3O2	O6-N2-C6	-7.30	109.99	119.80
2	C	1801	3O2	C6-C1-S1	7.05	112.55	107.25
2	D	1801	3O2	O6-N2-C6	-6.64	110.89	119.80
2	A	1801	3O2	O6-N2-C6	-6.47	111.11	119.80
2	D	1801	3O2	C6-C1-S1	6.37	112.04	107.25
2	A	1801	3O2	C19-N6-N3	-6.34	99.19	103.30
2	B	1801	3O2	C19-N6-N3	-6.32	99.20	103.30
2	C	1801	3O2	C19-N6-N3	-6.23	99.26	103.30
2	D	1801	3O2	C19-N6-N3	-5.85	99.50	103.30
2	B	1801	3O2	C6-C1-S1	5.73	111.56	107.25
2	A	1801	3O2	C17-C18-N3	-4.95	106.55	112.58
2	A	1801	3O2	C6-C1-S1	4.72	110.80	107.25
6	A	400	EPE	O2S-S-C10	4.22	110.42	106.81
2	C	1801	3O2	C16-O4-C11	-4.03	107.69	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1801	3O2	N5-N4-N3	-4.00	103.42	106.90
2	A	1801	3O2	C16-O4-C11	-3.69	108.53	117.94
2	B	1801	3O2	C4-C3-N1	-3.68	107.55	110.96
2	C	1801	3O2	N5-N4-N3	-3.51	103.84	106.90
2	A	1801	3O2	C4-C3-N1	-3.45	107.77	110.96
6	B	400	EPE	O2S-S-C10	3.37	109.69	106.81
6	B	400	EPE	O1S-S-C10	3.28	109.62	106.81
6	A	400	EPE	O1S-S-C10	3.25	109.59	106.81
2	B	1801	3O2	N5-N4-N3	-3.21	104.10	106.90
2	D	1801	3O2	N5-N4-N3	-3.17	104.14	106.90
2	B	1801	3O2	O2-S1-C10	-3.12	104.51	108.23
2	C	1801	3O2	C4-C3-N1	-3.11	108.08	110.96
2	D	1801	3O2	O3-S1-C10	-2.99	104.67	108.23
2	B	1801	3O2	C16-O4-C11	-2.99	110.32	117.94
2	C	1801	3O2	C17-C18-N3	-2.97	108.96	112.58
6	B	400	EPE	O3S-S-C10	2.87	109.57	105.93
2	D	1801	3O2	C16-O4-C11	-2.86	110.65	117.94
2	B	1801	3O2	C17-C18-N3	-2.79	109.18	112.58
2	B	1801	3O2	C5-C2-N1	-2.75	108.41	110.96
2	C	1801	3O2	O3-S1-C10	-2.73	104.98	108.23
2	A	1801	3O2	O3-S1-C10	-2.71	105.00	108.23
2	D	1801	3O2	O3-S1-C1	2.57	110.72	107.65
2	B	1801	3O2	N6-C19-N5	2.54	113.54	111.91
2	D	1801	3O2	C17-C18-N3	-2.46	109.58	112.58
2	D	1801	3O2	O2-S1-C10	-2.34	105.44	108.23
2	A	1801	3O2	O3-S1-C1	2.32	110.42	107.65
2	C	1801	3O2	C1-C6-N2	-2.27	112.56	116.33
2	D	1801	3O2	C4-C3-N1	-2.26	108.87	110.96
2	B	1801	3O2	O3-S1-C10	-2.24	105.56	108.23
2	A	1801	3O2	C5-C2-N1	-2.22	108.91	110.96
2	B	1801	3O2	C8-C7-N1	-2.21	107.13	113.20
2	C	1801	3O2	N6-C19-N5	2.20	113.32	111.91
2	C	1801	3O2	C5-C2-N1	-2.19	108.93	110.96
2	D	1801	3O2	N6-C19-N5	2.18	113.31	111.91
2	B	1801	3O2	C26-O7-C21	-2.10	110.11	118.83
2	A	1801	3O2	O2-S1-C10	-2.09	105.74	108.23
2	A	1801	3O2	C12-C10-S1	-2.05	117.58	119.40

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	164/164 (100%)	0.33	11 (6%) 17 17	4, 9, 20, 25	0
1	B	164/164 (100%)	0.46	14 (8%) 11 10	4, 9, 22, 27	0
1	C	164/164 (100%)	0.39	12 (7%) 15 14	5, 9, 17, 24	0
1	D	164/164 (100%)	0.41	12 (7%) 15 14	5, 9, 18, 27	0
All	All	656/656 (100%)	0.40	49 (7%) 16 14	4, 9, 20, 27	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2248	GLY	8.9
1	B	2249	LYS	8.6
1	B	2247	THR	7.6
1	D	2249	LYS	7.4
1	D	2246	TYR	7.3
1	B	2251	HIS	6.7
1	C	1250	SER	6.6
1	B	2250	SER	5.8
1	B	2109	ARG	5.5
1	C	1251	HIS	5.4
1	D	2247	THR	5.1
1	C	1104	ALA	5.0
1	B	2111	LEU	5.0
1	A	1111	LEU	5.0
1	D	2250	SER	4.9
1	C	1247	THR	4.9
1	A	1250	SER	4.8
1	A	1109	ARG	4.5
1	A	1251	HIS	4.5
1	C	1211	SER	4.3
1	A	1249	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1110	THR	3.9
1	A	1248	GLY	3.9
1	D	2251	HIS	3.8
1	C	1249	LYS	3.8
1	C	1248	GLY	3.4
1	A	1104	ALA	3.2
1	B	2248	GLY	3.2
1	A	1108	PRO	3.1
1	C	1267	GLY	3.1
1	B	2110	THR	2.7
1	D	2109	ARG	2.7
1	D	2212	LYS	2.7
1	B	2108	PRO	2.7
1	C	1212	LYS	2.7
1	B	2267	GLY	2.6
1	B	2195	TYR	2.6
1	C	1253	MET	2.5
1	A	1194	ASN	2.4
1	C	1109	ARG	2.3
1	D	2267	GLY	2.3
1	B	2194	ASN	2.2
1	D	2245	THR	2.2
1	D	2253	MET	2.2
1	C	1246	TYR	2.1
1	D	2110	THR	2.1
1	B	2260	GLN	2.1
1	A	1267	GLY	2.0
1	B	2234	LYS	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
6	EPE	B	400	12/15	0.16	4.05	37,37,37,37	0
6	EPE	A	400	12/15	0.17	3.50	29,29,30,30	0
5	SO4	B	3	5/5	0.15	2.49	45,45,46,46	0
5	SO4	A	9	5/5	0.15	2.00	47,48,48,48	0
4	CA	C	1996	1/1	0.14	1.83	35,35,35,35	0
4	CA	D	2996	1/1	0.13	1.22	37,37,37,37	0
3	ZN	B	2999	1/1	0.12	1.21	14,14,14,14	0
3	ZN	B	2998	1/1	0.12	1.16	13,13,13,13	0
5	SO4	A	2	5/5	0.12	0.79	47,47,48,48	0
5	SO4	C	1	5/5	0.14	0.44	41,41,41,42	0
2	3O2	A	1801	43/43	0.14	0.36	11,15,20,24	0
3	ZN	D	2998	1/1	0.11	0.29	12,12,12,12	0
5	SO4	D	8	5/5	0.16	0.17	33,33,34,34	0
3	ZN	D	2999	1/1	0.12	0.16	11,11,11,11	0
4	CA	B	2996	1/1	0.13	0.03	34,34,34,34	0
5	SO4	B	4	5/5	0.12	-0.01	39,39,39,40	0
2	3O2	B	1801	43/43	0.18	-0.07	19,28,50,51	0
2	3O2	C	1801	43/43	0.14	-0.13	12,17,22,26	0
4	CA	A	1996	1/1	0.11	-0.16	37,37,37,37	0
2	3O2	D	1801	43/43	0.15	-0.20	15,22,30,31	0
5	SO4	D	5	5/5	0.10	-0.40	36,36,36,36	0
5	SO4	A	7	5/5	0.12	-0.67	45,46,46,46	0
5	SO4	B	6	5/5	0.11	-0.80	40,41,41,41	0
4	CA	A	1997	1/1	0.05	-1.61	6,6,6,6	0
4	CA	B	2997	1/1	0.06	-1.94	11,11,11,11	0
3	ZN	A	1998	1/1	0.08	-2.18	8,8,8,8	0
3	ZN	C	1999	1/1	0.06	-2.37	9,9,9,9	0
3	ZN	A	1999	1/1	0.07	-2.45	8,8,8,8	0
4	CA	D	2997	1/1	0.04	-2.55	7,7,7,7	0
4	CA	C	1997	1/1	0.03	-3.28	8,8,8,8	0
3	ZN	C	1998	1/1	0.08	-3.99	8,8,8,8	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.