



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:00 PM GMT

PDB ID : 3H2C  
Title : Structural Studies of Pterin-Based Inhibitors of Dihydropteroate Synthase  
Authors : Yun, M.-K.; White, S.W.  
Deposited on : 2009-04-14  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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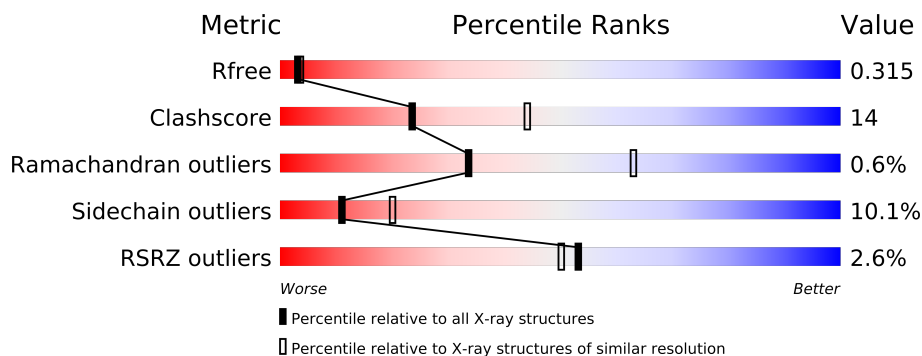
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1718 (2.60-2.60)
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  $\geq 3$ , 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	297	
1	B	297	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4132 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 Dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1986	1249	340	381	16			
1	B	263	Total	C	N	O	S	0	2	0
			2036	1283	348	387	18			

There are 40 discrepancies between the modelled and reference sequences:

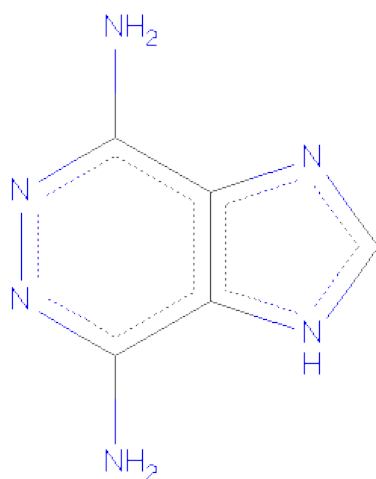
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP B1UXN2
A	-18	GLY	-	EXPRESSION TAG	UNP B1UXN2
A	-17	SER	-	EXPRESSION TAG	UNP B1UXN2
A	-16	SER	-	EXPRESSION TAG	UNP B1UXN2
A	-15	HIS	-	EXPRESSION TAG	UNP B1UXN2
A	-14	HIS	-	EXPRESSION TAG	UNP B1UXN2
A	-13	HIS	-	EXPRESSION TAG	UNP B1UXN2
A	-12	HIS	-	EXPRESSION TAG	UNP B1UXN2
A	-11	HIS	-	EXPRESSION TAG	UNP B1UXN2
A	-10	HIS	-	EXPRESSION TAG	UNP B1UXN2
A	-9	SER	-	EXPRESSION TAG	UNP B1UXN2
A	-8	SER	-	EXPRESSION TAG	UNP B1UXN2
A	-7	GLY	-	EXPRESSION TAG	UNP B1UXN2
A	-6	LEU	-	EXPRESSION TAG	UNP B1UXN2
A	-5	VAL	-	EXPRESSION TAG	UNP B1UXN2
A	-4	PRO	-	EXPRESSION TAG	UNP B1UXN2
A	-3	ARG	-	EXPRESSION TAG	UNP B1UXN2
A	-2	GLY	-	EXPRESSION TAG	UNP B1UXN2
A	-1	SER	-	EXPRESSION TAG	UNP B1UXN2
A	0	HIS	-	EXPRESSION TAG	UNP B1UXN2
B	-19	MET	-	EXPRESSION TAG	UNP B1UXN2
B	-18	GLY	-	EXPRESSION TAG	UNP B1UXN2
B	-17	SER	-	EXPRESSION TAG	UNP B1UXN2
B	-16	SER	-	EXPRESSION TAG	UNP B1UXN2
B	-15	HIS	-	EXPRESSION TAG	UNP B1UXN2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP B1UXN2
B	-13	HIS	-	EXPRESSION TAG	UNP B1UXN2
B	-12	HIS	-	EXPRESSION TAG	UNP B1UXN2
B	-11	HIS	-	EXPRESSION TAG	UNP B1UXN2
B	-10	HIS	-	EXPRESSION TAG	UNP B1UXN2
B	-9	SER	-	EXPRESSION TAG	UNP B1UXN2
B	-8	SER	-	EXPRESSION TAG	UNP B1UXN2
B	-7	GLY	-	EXPRESSION TAG	UNP B1UXN2
B	-6	LEU	-	EXPRESSION TAG	UNP B1UXN2
B	-5	VAL	-	EXPRESSION TAG	UNP B1UXN2
B	-4	PRO	-	EXPRESSION TAG	UNP B1UXN2
B	-3	ARG	-	EXPRESSION TAG	UNP B1UXN2
B	-2	GLY	-	EXPRESSION TAG	UNP B1UXN2
B	-1	SER	-	EXPRESSION TAG	UNP B1UXN2
B	0	HIS	-	EXPRESSION TAG	UNP B1UXN2

- Molecule 2 is 1H-IMIDAZO[4,5-D]PYRIDAZINE-4,7-DIAMINE (three-letter code: B58) (formula: C<sub>5</sub>H<sub>6</sub>N<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			11	5	6		
2	B	1	Total	C	N	0	0
			11	5	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	16	Total	O	0	0
			16	16		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.67Å 97.67Å 263.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.02 – 2.60 48.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.02-2.60) 88.3 (48.02-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.246 , 0.298 0.268 , 0.315	Depositor DCC
$R_{free}$ test set	1318 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.915	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	8 of 26446 reflections (0.030%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	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 47.68 % 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 9.5856e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: B58, 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	1.30	12/2012 (0.6%)	1.17	12/2711 (0.4%)
1	B	1.06	4/2071 (0.2%)	1.05	6/2794 (0.2%)
All	All	1.18	16/4083 (0.4%)	1.11	18/5505 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	LYS	CE-NZ	13.45	1.82	1.49
1	A	38	SER	CB-OG	7.74	1.52	1.42
1	A	198	GLU	CD-OE1	7.36	1.33	1.25
1	A	245	GLY	N-CA	6.87	1.56	1.46
1	A	93	GLU	CD-OE1	6.52	1.32	1.25
1	A	251	GLU	CD-OE1	5.88	1.32	1.25
1	A	194	GLU	CG-CD	5.51	1.60	1.51
1	A	249	GLY	C-O	-5.41	1.15	1.23
1	A	233	GLU	CD-OE2	5.36	1.31	1.25
1	B	-7	GLY	N-CA	5.35	1.54	1.46
1	B	50	LYS	CA-CB	5.33	1.65	1.53
1	A	274	LYS	CE-NZ	5.28	1.62	1.49
1	A	205	GLN	CB-CG	-5.26	1.38	1.52
1	B	250[A]	CYS	CB-SG	-5.21	1.73	1.81
1	B	250[B]	CYS	CB-SG	-5.21	1.73	1.81
1	A	259	LYS	CD-CE	5.07	1.64	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ASP	CB-CG-OD1	10.47	127.72	118.30
1	A	263	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	A	148	ARG	NE-CZ-NH2	-9.08	115.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	B	148	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	A	148	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	184	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	B	148	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	184	ASP	CB-CG-OD1	-7.01	111.99	118.30
1	A	184	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	184	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	8	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	21	LEU	CA-CB-CG	-5.27	103.19	115.30
1	A	250	CYS	CA-CB-SG	-5.19	104.65	114.00
1	B	271	MET	CG-SD-CE	5.15	108.44	100.20
1	A	244	LEU	CA-CB-CG	-5.08	103.62	115.30
1	A	271	MET	CG-SD-CE	-5.07	92.09	100.20
1	A	228	ASP	CB-CG-OD1	-5.02	113.78	118.30

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	1986	0	1981	67	0
1	B	2036	0	2039	51	0
2	A	11	0	6	0	0
2	B	11	0	6	1	0
3	A	25	0	0	1	0
3	B	30	0	0	0	0
4	A	17	0	0	0	0
4	B	16	0	0	0	0
All	All	4132	0	4032	117	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 14.

All (117) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:95:LYS:NZ	1:A:95:LYS:CE	1.82	1.41
1:A:212:PRO:HA	1:A:251:GLU:OE2	1.65	0.96
1:B:165[A]:TYR:CE1	1:B:209:LEU:HD22	2.05	0.91
1:B:214:LEU:HD12	1:B:252:PHE:CB	2.02	0.90
1:A:119:ILE:HG22	1:A:120:ASN:N	1.87	0.90
1:A:177:ARG:NH1	1:A:179:GLU:HG3	1.94	0.82
1:A:119:ILE:HG22	1:A:120:ASN:H	1.45	0.80
1:B:214:LEU:HD12	1:B:252:PHE:HB3	1.66	0.78
1:B:23:MET:HE1	1:B:254:ARG:HD2	1.64	0.78
1:B:214:LEU:HD12	1:B:252:PHE:HB2	1.64	0.78
1:B:28:VAL:O	1:B:30:PRO:HD3	1.89	0.72
1:A:144:LEU:HD13	1:A:167:SER:HB3	1.70	0.72
1:B:247:GLU:C	1:B:247:GLU:OE1	2.29	0.71
1:B:63:GLY:HA2	1:B:101:ASP:HB3	1.73	0.69
1:A:119:ILE:CG2	1:A:120:ASN:H	2.06	0.69
1:B:23:MET:CE	1:B:254:ARG:HD2	2.23	0.69
1:A:156:LEU:HG	1:A:160:MET:CE	2.24	0.68
1:B:14:LEU:HD21	1:B:97:PRO:HG2	1.76	0.68
1:A:119:ILE:CG2	1:A:120:ASN:N	2.55	0.67
1:A:252:PHE:N	1:A:252:PHE:CD1	2.61	0.67
1:B:18:GLU:HG3	1:B:19:LYS:HG2	1.75	0.66
1:B:227:LEU:HB3	1:B:229:LEU:HD12	1.79	0.65
1:B:220:LYS:NZ	2:B:902:B58:HN9	1.95	0.65
1:B:22:ILE:H	1:B:58:HIS:HD1	1.43	0.64
1:A:110:GLN:O	1:A:113:GLU:HB3	1.97	0.64
1:B:214:LEU:CD1	1:B:252:PHE:HB3	2.29	0.63
1:B:23:MET:HB2	1:B:59:ILE:HB	1.81	0.63
1:B:145:MET:HA	1:B:184:ASP:HB3	1.81	0.62
1:B:247:GLU:O	1:B:247:GLU:OE1	2.17	0.62
1:A:225:HIS:HD1	1:A:225:HIS:C	2.03	0.61
1:A:39:TYR:CD1	1:B:42:VAL:HB	2.36	0.61
1:A:23:MET:HB3	1:A:254:ARG:HA	1.82	0.60
1:B:214:LEU:CD1	1:B:252:PHE:CB	2.79	0.60
1:B:65:GLU:HG2	1:B:66:SER:N	2.18	0.59
1:A:214:LEU:HD11	1:A:254:ARG:HB2	1.85	0.59
1:A:91:SER:HB3	1:A:98:ILE:HD13	1.84	0.59
1:A:206:LEU:HD12	1:A:206:LEU:N	2.19	0.57
1:A:63:GLY:HA2	1:A:101:ASP:HB3	1.87	0.57
1:A:156:LEU:CD2	1:A:198:GLU:HG2	2.35	0.56
1:A:204:GLU:O	1:A:207:ASN:HB2	2.04	0.56
1:A:227:LEU:HB3	1:A:229:LEU:HD12	1.88	0.56
1:A:51:GLU:O	1:A:55:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:51:GLU:O	1:B:55:GLU:HG2	2.06	0.54
1:B:53:ARG:NH1	1:B:54:ASP:OD1	2.40	0.54
1:B:51:GLU:O	1:B:55:GLU:CG	2.56	0.54
1:A:95:LYS:NZ	1:A:95:LYS:CD	2.68	0.53
1:A:22:ILE:HD12	1:A:253:VAL:HG22	1.91	0.53
1:A:187:ILE:HG21	1:A:217:THR:HG22	1.91	0.53
1:A:86:MET:O	1:A:90:VAL:HG23	2.08	0.52
1:A:214:LEU:HD13	1:A:252:PHE:HB2	1.90	0.52
1:A:236:GLU:CD	1:A:236:GLU:H	2.13	0.52
1:A:108:ALA:O	1:A:112:ILE:HD12	2.09	0.52
1:A:156:LEU:HG	1:A:160:MET:HE3	1.91	0.52
1:A:211:TYR:HB3	1:A:212:PRO:HD2	1.91	0.51
1:A:204:GLU:OE2	1:A:204:GLU:N	2.36	0.51
1:B:12:TYR:CB	1:B:97:PRO:HG3	2.41	0.51
1:A:95:LYS:O	1:A:96:LEU:HD23	2.10	0.51
1:B:165[A]:TYR:CZ	1:B:209:LEU:HD22	2.45	0.50
1:A:6:ASP:OD1	1:A:15:ASN:HA	2.11	0.49
1:A:121:ASP:OD2	1:A:121:ASP:C	2.50	0.49
1:B:61:ASP:OD2	1:B:99:SER:OG	2.31	0.49
1:A:38:SER:OG	1:A:41:GLU:HG3	2.13	0.49
1:A:53:ARG:NH1	1:A:54:ASP:OD1	2.46	0.49
1:A:120:ASN:HA	1:A:143:ILE:HB	1.95	0.48
1:A:225:HIS:ND1	1:A:225:HIS:C	2.64	0.48
1:A:206:LEU:HD12	1:A:206:LEU:H	1.79	0.48
1:A:268:MET:HA	1:A:271:MET:CE	2.42	0.48
1:A:225:HIS:ND1	1:A:225:HIS:O	2.47	0.47
1:B:187:ILE:HG21	1:B:217:THR:HG22	1.97	0.47
1:A:228:ASP:O	1:A:229:LEU:HG	2.14	0.47
1:B:129:PRO:O	1:B:131:ILE:N	2.48	0.47
1:B:83:VAL:O	1:B:87:ILE:HG13	2.15	0.47
1:B:83:VAL:O	1:B:86:MET:HB2	2.15	0.46
1:A:259:LYS:HB3	1:A:259:LYS:HE2	1.75	0.46
1:A:110:GLN:O	1:A:114:ALA:N	2.49	0.45
1:B:224:GLY:O	1:B:228:ASP:HA	2.17	0.45
1:B:165[A]:TYR:HE1	1:B:209:LEU:HD22	1.72	0.45
1:A:131:ILE:CG2	1:A:132:ALA:N	2.80	0.45
1:A:131:ILE:O	1:A:134:VAL:HB	2.17	0.44
1:B:119:ILE:HG22	1:B:120:ASN:N	2.31	0.44
1:A:218:SER:HB3	1:A:256:HIS:ND1	2.31	0.44
1:B:214:LEU:CD1	1:B:252:PHE:HB2	2.42	0.44
1:A:254:ARG:NH2	3:A:278:SO4:O3	2.42	0.44
1:A:228:ASP:C	1:A:228:ASP:OD1	2.56	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:28:VAL:O	1:B:30:PRO:CD	2.63	0.44
1:A:131:ILE:HG23	1:A:132:ALA:N	2.32	0.44
1:B:86:MET:O	1:B:90:VAL:HG23	2.18	0.44
1:B:176:VAL:HG12	1:B:177:ARG:O	2.18	0.43
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.76	0.43
1:A:185:PRO:HG3	1:A:203:LEU:HD21	2.01	0.43
1:B:227:LEU:HA	1:B:227:LEU:HD23	1.80	0.43
1:B:134:VAL:HG12	1:B:138:TYR:HD2	1.83	0.43
1:A:23:MET:SD	1:A:254:ARG:HG3	2.59	0.43
1:A:211:TYR:HB3	1:A:212:PRO:CD	2.48	0.43
1:A:189:PHE:CD1	1:A:189:PHE:N	2.86	0.43
1:A:271:MET:HB2	1:A:271:MET:HE3	1.92	0.43
1:B:80:ILE:O	1:B:81:LYS:C	2.58	0.43
1:B:148:ARG:HD2	1:B:153:TYR:CZ	2.53	0.42
1:B:185:PRO:HD2	1:B:214:LEU:O	2.19	0.42
1:B:28:VAL:HG21	1:B:63:GLY:O	2.19	0.42
1:B:130:LYS:HA	1:B:133:GLU:HG3	2.01	0.42
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.77	0.42
1:A:84:VAL:HB	1:A:85:PRO:HD3	2.02	0.42
1:A:91:SER:HA	1:A:98:ILE:HD11	2.02	0.41
1:A:156:LEU:HD23	1:A:198:GLU:HG2	2.02	0.41
1:A:17:ASN:O	1:A:274:LYS:HG3	2.20	0.41
1:B:86:MET:H	1:B:86:MET:HG2	1.68	0.41
1:B:230:PRO:HD2	1:B:233:GLU:HG3	2.02	0.41
1:A:79:GLU:O	1:A:83:VAL:HB	2.20	0.41
1:B:232:GLU:OE1	1:B:232:GLU:N	2.51	0.41
1:B:53:ARG:NH1	1:B:53:ARG:HB3	2.36	0.40
1:A:135:ALA:O	1:A:136:ALA:C	2.59	0.40
1:A:4:ASP:N	1:A:4:ASP:OD2	2.54	0.40
1:A:156:LEU:HD22	1:A:198:GLU:HG2	2.02	0.40
1:B:53:ARG:HB3	1:B:53:ARG:HH11	1.85	0.40
1:A:244:LEU:HG	1:A:244:LEU:O	2.21	0.40
1:A:206:LEU:N	1:A:206:LEU:CD1	2.84	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	249/297 (84%)	224 (90%)	24 (10%)	1 (0%)	43	72
1	B	257/297 (86%)	230 (90%)	25 (10%)	2 (1%)	27	53
All	All	506/594 (85%)	454 (90%)	49 (10%)	3 (1%)	33	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	130	LYS
1	A	219	ARG
1	B	29	THR

### 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	210/247 (85%)	186 (89%)	24 (11%)	8	15
1	B	216/247 (87%)	197 (91%)	19 (9%)	14	27
All	All	426/494 (86%)	383 (90%)	43 (10%)	11	20

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	GLU
1	A	22	ILE
1	A	41	GLU
1	A	78	GLU
1	A	80	ILE
1	A	82	ARG
1	A	88	GLN
1	A	92	LYS
1	A	117	HIS
1	A	139	ASP
1	A	140	VAL

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Mol	Chain	Res	Type
1	A	151	MET
1	A	179	GLU
1	A	187	ILE
1	A	197	LEU
1	A	198	GLU
1	A	200	MET
1	A	218	SER
1	A	219	ARG
1	A	235	LEU
1	A	244	LEU
1	A	252	PHE
1	A	257	ASP
1	B	1	MET
1	B	7	LEU
1	B	9	CYS
1	B	53	ARG
1	B	55	GLU
1	B	65	GLU
1	B	83	VAL
1	B	122	ILE
1	B	139	ASP
1	B	150	ASN
1	B	155	ASN
1	B	178	ASP
1	B	203	LEU
1	B	206	LEU
1	B	212	PRO
1	B	220	LYS
1	B	247	GLU
1	B	261	MET
1	B	271	MET

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	110	GLN
1	A	180	ASN
1	B	48	HIS
1	B	152	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 ⓘ

13 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	$\# Z  > 2$
3	SO4	A	278	-	4,4,4	0.86	0	6,6,6	0.79	0
3	SO4	A	279	-	4,4,4	0.19	0	6,6,6	0.50	0
3	SO4	A	280	-	4,4,4	0.26	0	6,6,6	0.57	0
3	SO4	A	281	-	4,4,4	0.61	0	6,6,6	0.43	0
3	SO4	A	282	-	4,4,4	0.66	0	6,6,6	0.39	0
2	B58	A	901	-	12,12,12	1.51	2 (16%)	16,17,17	1.23	1 (6%)
3	SO4	B	278	-	4,4,4	0.34	0	6,6,6	0.54	0
3	SO4	B	279	-	4,4,4	0.43	0	6,6,6	0.63	0
3	SO4	B	280	-	4,4,4	0.21	0	6,6,6	0.34	0
3	SO4	B	281	-	4,4,4	0.22	0	6,6,6	0.59	0
3	SO4	B	282	-	4,4,4	0.49	0	6,6,6	0.52	0
3	SO4	B	283	-	4,4,4	0.44	0	6,6,6	0.95	1 (16%)
2	B58	B	902	-	12,12,12	1.42	2 (16%)	16,17,17	1.79	4 (25%)

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
3	SO4	A	278	-	-	0/0/0/0	0/0/0/0
3	SO4	A	279	-	-	0/0/0/0	0/0/0/0
3	SO4	A	280	-	-	0/0/0/0	0/0/0/0
3	SO4	A	281	-	-	0/0/0/0	0/0/0/0
3	SO4	A	282	-	-	0/0/0/0	0/0/0/0
2	B58	A	901	-	-	0/0/0/0	0/0/2/2
3	SO4	B	278	-	-	0/0/0/0	0/0/0/0
3	SO4	B	279	-	-	0/0/0/0	0/0/0/0
3	SO4	B	280	-	-	0/0/0/0	0/0/0/0
3	SO4	B	281	-	-	0/0/0/0	0/0/0/0
3	SO4	B	282	-	-	0/0/0/0	0/0/0/0
3	SO4	B	283	-	-	0/0/0/0	0/0/0/0
2	B58	B	902	-	-	0/0/0/0	0/0/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	B58	N2-N1	3.48	1.43	1.34
2	B	902	B58	N2-N1	3.19	1.42	1.34
2	A	901	B58	C3-C4	2.68	1.50	1.44
2	B	902	B58	C5-N7	-2.32	1.31	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	B58	C6-N1-N2	3.70	125.52	119.91
2	B	902	B58	C8-N9-C4	-3.32	106.16	108.52
2	B	902	B58	C4-C3-N2	-2.57	117.78	122.54
2	A	901	B58	C6-N1-N2	2.23	123.29	119.91
2	B	902	B58	C5-C4-N9	2.08	107.76	106.07
3	B	283	SO4	O2-S-O1	-2.03	102.83	109.53

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	257/297 (86%)	0.47	7 (2%)	52	49	30, 57, 69, 93	0
1	B	263/297 (88%)	0.44	7 (2%)	52	49	48, 61, 74, 97	0
All	All	520/594 (87%)	0.45	14 (2%)	53	49	30, 59, 74, 97	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	GLU	4.0
1	B	106	GLU	3.9
1	B	79	GLU	3.2
1	B	75	SER	3.0
1	A	37	GLY	2.9
1	A	7	LEU	2.8
1	B	30	PRO	2.7
1	A	9	CYS	2.6
1	A	39	TYR	2.4
1	B	18	GLU	2.3
1	B	78	GLU	2.2
1	A	65	GLU	2.1
1	A	92	LYS	2.1
1	B	223	ILE	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
3	SO4	A	280	5/5	0.25	1.05	84,85,86,88	0
3	SO4	B	280	5/5	0.21	0.45	106,107,107,108	0
3	SO4	A	282	5/5	0.16	-1.26	101,101,102,104	0
3	SO4	B	281	5/5	0.18	-1.35	99,99,99,100	0
3	SO4	B	282	5/5	0.13	-1.43	95,97,97,99	0
3	SO4	B	283	5/5	0.14	-1.62	98,98,99,101	0
2	B58	B	902	11/11	0.14	-1.82	47,49,50,52	0
3	SO4	B	279	5/5	0.10	-2.14	88,89,90,91	0
3	SO4	B	278	5/5	0.12	-2.20	68,69,69,70	0
3	SO4	A	278	5/5	0.14	-2.21	57,58,60,61	0
2	B58	A	901	11/11	0.12	-2.50	47,48,48,49	0
3	SO4	A	281	5/5	0.14	-2.59	84,85,87,88	0
3	SO4	A	279	5/5	0.10	-3.96	86,87,88,90	0

## 6.5 Other polymers

There are no such residues in this entry.