



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:58 PM GMT

PDB ID : 1H5N  
Title : DMSO REDUCTASE MODIFIED BY THE PRESENCE OF DMS AND AIR  
Authors : Bailey, S.; Adams, B.; Smith, A.T.; Richards, R.L.; Lowe, D.J.; Bray, R.C.  
Deposited on : 2001-05-22  
Resolution : 2.00 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>

---

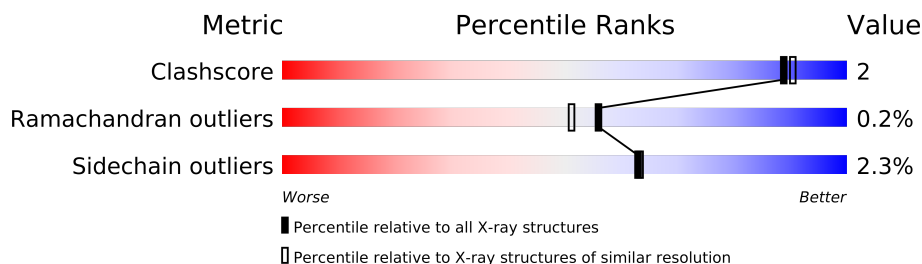
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	823	
1	C	823	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13178 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 DMSO REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			5867	3730	994	1116	27			
1	C	766	Total	C	N	O	S	0	0	0
			5877	3737	995	1118	27			

There are 26 discrepancies between the modelled and reference sequences:

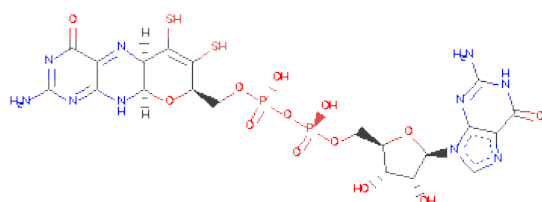
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	SER	THR	SEQUENCED FROM MAP	UNP Q52675
A	43	ALA	GLU	SEQUENCED FROM MAP	UNP Q52675
A	107	GLU	GLN	SEQUENCED FROM MAP	UNP Q52675
A	234	GLU	ASP	SEQUENCED FROM MAP	UNP Q52675
A	236	ILE	VAL	SEQUENCED FROM MAP	UNP Q52675
A	280	ASP	MET	SEQUENCED FROM MAP	UNP Q52675
A	294	GLU	SER	SEQUENCED FROM MAP	UNP Q52675
A	295	GLY	ASP	SEQUENCED FROM MAP	UNP Q52675
A	312	GLU	ILE	SEQUENCED FROM MAP	UNP Q52675
A	374	ALA	SER	SEQUENCED FROM MAP	UNP Q52675
A	456	VAL	ILE	SEQUENCED FROM MAP	UNP Q52675
A	526	ALA	LYS	SEQUENCED FROM MAP	UNP Q52675
A	555	GLN	GLU	SEQUENCED FROM MAP	UNP Q52675
C	39	SER	THR	SEQUENCED FROM MAP	UNP Q52675
C	43	ALA	GLU	SEQUENCED FROM MAP	UNP Q52675
C	107	GLU	GLN	SEQUENCED FROM MAP	UNP Q52675
C	234	GLU	ASP	SEQUENCED FROM MAP	UNP Q52675
C	236	ILE	VAL	SEQUENCED FROM MAP	UNP Q52675
C	280	ASP	MET	SEQUENCED FROM MAP	UNP Q52675
C	294	GLU	SER	SEQUENCED FROM MAP	UNP Q52675
C	295	GLY	ASP	SEQUENCED FROM MAP	UNP Q52675
C	312	GLU	ILE	SEQUENCED FROM MAP	UNP Q52675
C	374	ALA	SER	SEQUENCED FROM MAP	UNP Q52675
C	456	VAL	ILE	SEQUENCED FROM MAP	UNP Q52675
C	526	ALA	LYS	SEQUENCED FROM MAP	UNP Q52675

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	555	GLN	GLU	SEQUENCED FROM MAP	UNP Q52675

- Molecule 2 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONEGUANOSINE DINUCLEOTIDE (three-letter code: PGD) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
2	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 3 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	652	Total	O	0	0
			652	652		
5	C	582	Total	O	0	0
			582	582		

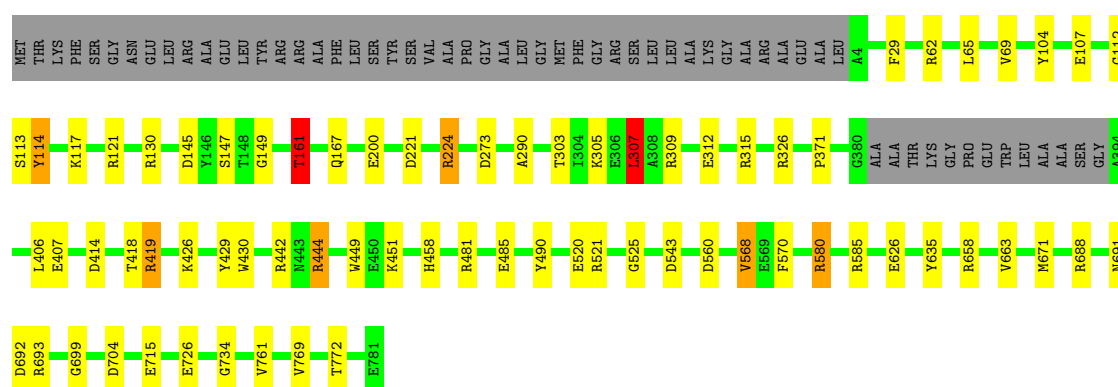
### 3 Residue-property plots

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.

Note EDS was not executed.

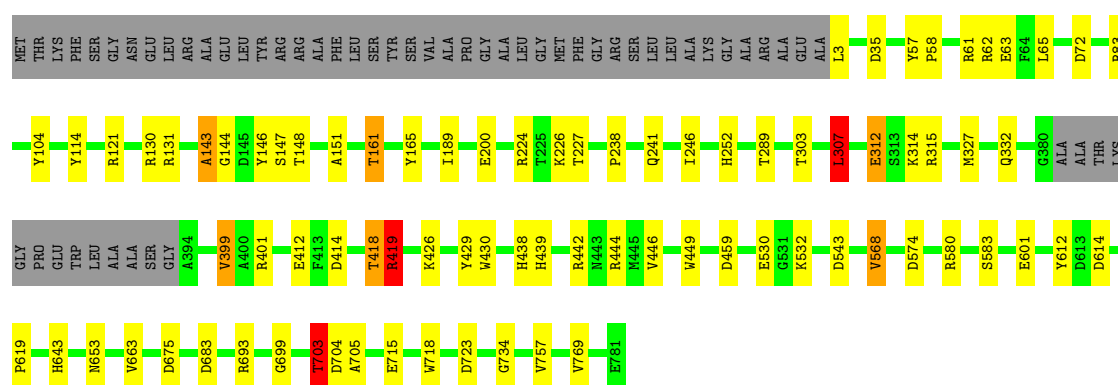
#### • Molecule 1: DMSO REDUCTASE

Chain A:



#### • Molecule 1: DMSO REDUCTASE

Chain C:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.80Å 116.10Å 230.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	83.7 (20.00-2.00)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.158 , 0.209	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MO, PGD, 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	0.67	1/6024 (0.0%)	1.35	49/8198 (0.6%)
1	C	0.64	1/6034 (0.0%)	1.34	50/8213 (0.6%)
All	All	0.66	2/12058 (0.0%)	1.34	99/16411 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	GLU	CD-OE1	-10.26	1.14	1.25
1	C	312	GLU	CD-OE1	-5.32	1.19	1.25

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	ARG	NE-CZ-NH2	-21.09	109.75	120.30
1	C	130	ARG	NE-CZ-NH1	-17.14	111.73	120.30
1	C	83	ARG	NE-CZ-NH1	15.10	127.85	120.30
1	A	62	ARG	NE-CZ-NH2	-14.14	113.23	120.30
1	A	224	ARG	NE-CZ-NH2	13.97	127.28	120.30
1	A	62	ARG	NE-CZ-NH1	13.63	127.12	120.30
1	C	62	ARG	NE-CZ-NH1	12.61	126.60	120.30
1	C	130	ARG	NE-CZ-NH2	12.51	126.55	120.30
1	A	312	GLU	OE1-CD-OE2	-11.58	109.41	123.30
1	A	224	ARG	CD-NE-CZ	11.27	139.38	123.60
1	A	658	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	A	326	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	C	312	GLU	OE1-CD-OE2	-9.63	111.75	123.30
1	C	401	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	A	312	GLU	CG-CD-OE2	9.14	136.58	118.30
1	A	273	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	521	ARG	NE-CZ-NH1	8.91	124.76	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	VAL	CB-CA-C	-8.77	94.74	111.40
1	A	419	ARG	CD-NE-CZ	8.62	135.67	123.60
1	A	688	ARG	CD-NE-CZ	8.54	135.56	123.60
1	A	419	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	130	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	A	543	ASP	CB-CG-OD1	8.25	125.72	118.30
1	A	307	LEU	CB-CG-CD2	8.19	124.92	111.00
1	A	444	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	C	83	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	C	224	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	A	130	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	A	442	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	C	568	VAL	CB-CA-C	-7.65	96.86	111.40
1	A	585	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	A	309	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	C	703	THR	CB-CA-C	-7.30	91.89	111.60
1	C	131	ARG	NE-CZ-NH1	-7.27	116.66	120.30
1	A	704	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	769	VAL	N-CA-CB	-7.25	95.55	111.50
1	C	574	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	C	312	GLU	CG-CD-OE2	7.15	132.60	118.30
1	A	568	VAL	N-CA-CB	6.99	126.88	111.50
1	A	568	VAL	CA-CB-CG2	6.95	121.32	110.90
1	A	692	ASP	CB-CG-OD1	6.78	124.41	118.30
1	A	688	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	543	ASP	CB-CG-OD1	6.73	124.36	118.30
1	C	442	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	C	35	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	C	683	ASP	CB-CG-OD1	6.65	124.28	118.30
1	C	601	GLU	OE1-CD-OE2	-6.61	115.37	123.30
1	C	580	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	C	165	TYR	CB-CG-CD2	6.46	124.88	121.00
1	C	568	VAL	CA-CB-CG2	6.28	120.32	110.90
1	C	568	VAL	N-CA-CB	6.22	125.19	111.50
1	A	580	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	61	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	A	693	ARG	CG-CD-NE	6.15	124.71	111.80
1	C	143	ALA	N-CA-CB	6.15	118.70	110.10
1	C	161	THR	CB-CA-C	-6.01	95.38	111.60
1	C	459	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	612	TYR	CB-CG-CD1	-6.00	117.40	121.00
1	C	446	VAL	CA-CB-CG2	-6.00	101.90	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	ARG	CD-NE-CZ	5.95	131.93	123.60
1	C	307	LEU	CA-CB-CG	5.94	128.95	115.30
1	A	114	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	C	114	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	C	114	TYR	O-C-N	5.86	133.16	123.20
1	A	560	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	485	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	C	63	GLU	CG-CD-OE2	-5.69	106.92	118.30
1	C	83	ARG	CD-NE-CZ	5.68	131.56	123.60
1	C	72	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	658	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
1	C	224	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	A	726	GLU	CG-CD-OE1	5.62	129.55	118.30
1	A	161	THR	N-CA-CB	5.56	120.86	110.30
1	A	419	ARG	CB-CA-C	-5.56	99.29	110.40
1	A	458	HIS	CA-CB-CG	5.55	123.04	113.60
1	C	693	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	114	TYR	CB-CG-CD2	5.52	124.31	121.00
1	A	29	PHE	CB-CG-CD1	5.50	124.65	120.80
1	C	121	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	444	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	481	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	315	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	C	704	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	612	TYR	CB-CG-CD2	5.42	124.25	121.00
1	A	626	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	C	57	TYR	CB-CG-CD1	5.36	124.22	121.00
1	C	675	ASP	CB-CG-OD2	5.34	123.10	118.30
1	C	757	VAL	CB-CA-C	-5.33	101.27	111.40
1	C	723	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	490	TYR	CB-CG-CD1	5.32	124.19	121.00
1	C	419	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	444	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	C	165	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	121	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	221	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	224	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	C	614	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	444	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	315	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	5867	0	5668	25	0
1	C	5877	0	5677	28	0
2	A	94	0	40	1	0
2	C	94	0	40	2	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	652	0	0	7	0
5	C	582	0	0	4	0
All	All	13178	0	11425	53	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 2.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:189:ILE:HD12	1:C:227:THR:HA	1.54	0.89
1:A:407:GLU:OE1	1:A:444:ARG:NH2	2.07	0.88
1:A:671:MET:HE1	1:A:761:VAL:HG11	1.65	0.76
1:A:147:SER:HA	2:A:1782:PGD:S13	2.28	0.73
1:A:149:GLY:HA2	5:A:2159:HOH:O	1.89	0.72
1:C:530:GLU:HG3	1:C:532:LYS:HZ3	1.60	0.66
1:C:147:SER:HA	2:C:1782:PGD:S13	2.37	0.65
1:C:414:ASP:OD1	1:C:419:ARG:HG2	1.98	0.64
1:C:144:GLY:HA3	5:C:2129:HOH:O	1.98	0.63
1:A:407:GLU:HG2	5:A:2354:HOH:O	2.00	0.60
1:A:414:ASP:OD1	1:A:419:ARG:HG2	2.01	0.59
1:C:314:LYS:NZ	5:C:2257:HOH:O	2.26	0.59
1:C:143:ALA:O	1:C:399:VAL:HG22	2.03	0.59
1:A:451:LYS:HG2	5:A:2372:HOH:O	2.05	0.56
1:A:772:THR:OG1	5:A:2640:HOH:O	2.18	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:530:GLU:HG3	1:C:532:LYS:NZ	2.22	0.55
1:C:703:THR:HG22	1:C:705:ALA:H	1.71	0.55
1:C:653:ASN:ND2	1:C:718:TRP:H	2.05	0.55
1:C:147:SER:HB3	2:C:1783:PGD:S12	2.49	0.53
1:C:146:TYR:HH	1:C:439:HIS:HD1	1.57	0.53
1:A:663:VAL:HB	1:A:699:GLY:HA3	1.93	0.51
1:A:224:ARG:HD2	5:A:2223:HOH:O	2.11	0.49
1:C:148:THR:HB	1:C:151:ALA:HB3	1.95	0.48
1:A:406:LEU:O	1:A:451:LYS:HD2	2.14	0.48
1:C:412:GLU:OE1	1:C:419:ARG:NH1	2.47	0.47
1:A:69:VAL:HG22	5:A:2019:HOH:O	2.15	0.47
1:A:114:TYR:OH	1:A:145:ASP:HB2	2.15	0.47
1:C:104:TYR:CE1	1:C:426:LYS:HG3	2.49	0.47
1:C:303:THR:O	1:C:307:LEU:HD22	2.15	0.47
1:A:107:GLU:H	1:A:107:GLU:CD	2.20	0.46
1:A:635:TYR:CZ	1:A:691:ASN:HA	2.51	0.46
1:A:303:THR:HG22	1:A:307:LEU:HD23	1.98	0.45
1:C:3:LEU:N	5:C:2001:HOH:O	2.48	0.45
1:C:303:THR:HG22	1:C:307:LEU:HD22	1.99	0.45
1:A:290:ALA:HB3	1:A:305:LYS:HE3	1.99	0.45
1:C:252:HIS:CE1	1:C:289:THR:HG22	2.52	0.45
1:C:418:THR:HG23	5:C:2300:HOH:O	2.16	0.45
1:A:671:MET:CE	1:A:761:VAL:HG11	2.41	0.45
1:C:104:TYR:CD1	1:C:426:LYS:HG3	2.53	0.44
1:A:161:THR:HG22	5:A:2169:HOH:O	2.18	0.43
1:C:663:VAL:HB	1:C:699:GLY:HA3	2.00	0.43
1:C:241:GLN:HG2	1:C:327:MET:SD	2.59	0.43
1:C:238:PRO:HB3	1:C:246:ILE:HD11	2.01	0.43
1:A:104:TYR:CE1	1:A:426:LYS:HG3	2.54	0.42
1:A:371:PRO:HD2	1:A:570:PHE:CZ	2.55	0.42
1:C:703:THR:CG2	1:C:705:ALA:H	2.32	0.42
1:A:167:GLN:O	1:A:580:ARG:HD2	2.20	0.42
1:A:114:TYR:CE1	1:A:145:ASP:HA	2.55	0.42
1:A:112:GLY:O	1:A:113:SER:C	2.58	0.42
1:A:520:GLU:OE1	1:A:525:GLY:HA3	2.21	0.41
1:C:332:GLN:OE1	1:C:619:PRO:HA	2.22	0.40
1:C:643:HIS:CD2	1:C:643:HIS:N	2.87	0.40
1:C:312:GLU:O	1:C:312:GLU:HG3	2.21	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	761/823 (92%)	735 (97%)	24 (3%)	2 (0%)	50	44
1	C	762/823 (93%)	740 (97%)	21 (3%)	1 (0%)	59	55
All	All	1523/1646 (92%)	1475 (97%)	45 (3%)	3 (0%)	56	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LYS
1	A	734	GLY
1	C	734	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	607/648 (94%)	597 (98%)	10 (2%)	75	77
1	C	608/648 (94%)	590 (97%)	18 (3%)	53	50
All	All	1215/1296 (94%)	1187 (98%)	28 (2%)	63	63

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	161	THR
1	A	200	GLU
1	A	307	LEU
1	A	418	THR
1	A	429	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	430	TRP
1	A	449	TRP
1	A	568	VAL
1	A	715	GLU
1	C	58	PRO
1	C	65	LEU
1	C	161	THR
1	C	200	GLU
1	C	226	LYS
1	C	307	LEU
1	C	399	VAL
1	C	418	THR
1	C	419	ARG
1	C	429	TYR
1	C	430	TRP
1	C	438	HIS
1	C	449	TRP
1	C	568	VAL
1	C	583	SER
1	C	703	THR
1	C	715	GLU
1	C	769	VAL

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	241	GLN
1	A	653	ASN
1	C	152	GLN
1	C	241	GLN
1	C	408	ASN
1	C	606	ASN
1	C	653	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PGD	A	1782	3	52,52,52	3.06	18 (34%)	72,81,81	3.54	14 (19%)
2	PGD	A	1783	3	52,52,52	3.06	19 (36%)	72,81,81	2.16	15 (20%)
4	SO4	A	1785	-	4,4,4	0.70	0	6,6,6	0.20	0
2	PGD	C	1782	3	52,52,52	3.18	16 (30%)	72,81,81	3.80	13 (18%)
2	PGD	C	1783	3	52,52,52	3.43	21 (40%)	72,81,81	2.52	15 (20%)
4	SO4	C	1785	-	4,4,4	0.87	0	6,6,6	0.30	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	PGD	A	1782	3	-	0/22/82/82	0/1/6/6
2	PGD	A	1783	3	-	0/22/82/82	0/1/6/6
4	SO4	A	1785	-	-	0/0/0/0	0/0/0/0
2	PGD	C	1782	3	-	0/22/82/82	0/1/6/6
2	PGD	C	1783	3	-	0/22/82/82	0/1/6/6
4	SO4	C	1785	-	-	0/0/0/0	0/0/0/0

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1783	PGD	C16-N15	16.98	1.47	1.28
2	C	1782	PGD	C16-N15	16.30	1.47	1.28
2	A	1782	PGD	C16-N15	14.46	1.45	1.28
2	A	1783	PGD	C16-N15	14.02	1.44	1.28
2	C	1783	PGD	C21-N22	8.85	1.44	1.35
2	A	1782	PGD	C21-N22	7.21	1.42	1.35
2	C	1782	PGD	C21-N22	6.75	1.42	1.35
2	A	1783	PGD	C2-N2	6.62	1.42	1.32
2	A	1783	PGD	C21-N22	6.52	1.41	1.35
2	C	1783	PGD	C2-N2	6.31	1.42	1.32
2	C	1782	PGD	C2-N2	6.12	1.41	1.32
2	A	1782	PGD	PA-O1A	5.96	1.74	1.51
2	C	1782	PGD	PA-O1A	5.56	1.72	1.51
2	A	1782	PGD	C2-N2	5.25	1.40	1.32
2	C	1783	PGD	PB-O1B	5.12	1.70	1.51
2	A	1783	PGD	PB-O1B	4.96	1.70	1.51
2	C	1782	PGD	PB-O1B	4.94	1.70	1.51
2	C	1783	PGD	PA-O1A	4.68	1.69	1.51
2	A	1783	PGD	PA-O1A	4.54	1.68	1.51
2	A	1782	PGD	PB-O1B	4.54	1.68	1.51
2	A	1782	PGD	C2-N3	3.97	1.38	1.33
2	A	1782	PGD	C19-N19	3.67	1.43	1.34
2	A	1783	PGD	C19-N19	3.65	1.42	1.34
2	A	1782	PGD	PB-O5'	3.63	1.75	1.59
2	C	1783	PGD	PA-O3A	3.53	1.75	1.59
2	A	1783	PGD	C10-C11	3.50	1.57	1.52
2	C	1783	PGD	C19-N19	3.45	1.42	1.34
2	C	1782	PGD	PB-O5'	3.44	1.74	1.59
2	A	1782	PGD	PA-O3A	3.42	1.74	1.59
2	C	1783	PGD	O11-C23	-3.39	1.39	1.44
2	C	1783	PGD	PB-O2B	3.38	1.70	1.55
2	C	1783	PGD	O4'-C1'	3.37	1.46	1.41
2	A	1783	PGD	PB-O5'	3.37	1.74	1.59
2	A	1783	PGD	PA-O3A	3.32	1.74	1.59
2	A	1783	PGD	PA-O2A	3.30	1.69	1.55
2	A	1783	PGD	C2-N3	3.27	1.37	1.33
2	C	1783	PGD	PB-O3B	3.26	1.65	1.59
2	C	1782	PGD	C17-C16	-3.13	1.38	1.47
2	A	1782	PGD	PB-O2B	3.12	1.69	1.55
2	C	1782	PGD	PA-O2A	3.11	1.68	1.55
2	C	1783	PGD	PA-O2A	3.08	1.68	1.55
2	A	1783	PGD	PB-O2B	3.01	1.68	1.55
2	C	1782	PGD	O4'-C1'	2.93	1.45	1.41

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1782	PGD	PA-O3A	2.85	1.72	1.59
2	C	1782	PGD	C2-N3	2.84	1.37	1.33
2	C	1782	PGD	PB-O2B	2.82	1.67	1.55
2	C	1782	PGD	C19-N19	2.78	1.40	1.34
2	A	1783	PGD	O11-C11	-2.77	1.39	1.43
2	A	1782	PGD	C17-C16	-2.75	1.39	1.47
2	C	1783	PGD	PB-O5'	2.70	1.71	1.59
2	A	1783	PGD	C14-N15	2.59	1.48	1.46
2	C	1783	PGD	C17-C16	-2.57	1.39	1.47
2	C	1783	PGD	O11-C11	-2.54	1.39	1.43
2	A	1782	PGD	C10-C11	2.51	1.55	1.52
2	C	1783	PGD	C2-N3	2.50	1.36	1.33
2	A	1783	PGD	PA-O3B	2.47	1.64	1.59
2	A	1782	PGD	PA-O3B	2.46	1.64	1.59
2	C	1783	PGD	C4-N9	-2.45	1.34	1.37
2	A	1782	PGD	PA-O2A	2.44	1.65	1.55
2	A	1782	PGD	PB-O3B	2.35	1.64	1.59
2	A	1782	PGD	C5-C4	-2.34	1.35	1.40
2	A	1783	PGD	C4-N9	-2.33	1.34	1.37
2	A	1783	PGD	O11-C23	-2.31	1.40	1.44
2	A	1783	PGD	C21-N20	2.28	1.38	1.32
2	A	1782	PGD	C12-S12	2.19	1.82	1.74
2	C	1782	PGD	C10-C11	2.18	1.55	1.52
2	A	1783	PGD	C17-C16	-2.18	1.40	1.47
2	C	1783	PGD	C12-S12	2.18	1.82	1.74
2	C	1782	PGD	C4-N9	-2.13	1.34	1.37
2	A	1782	PGD	C14-N15	2.11	1.48	1.46
2	C	1783	PGD	C19-N18	2.10	1.38	1.35
2	C	1783	PGD	C21-N20	2.07	1.37	1.32
2	C	1783	PGD	C5-C4	-2.07	1.35	1.40
2	C	1782	PGD	C13-S13	2.05	1.82	1.74

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1782	PGD	C6-C5-N7	-28.60	130.29	134.14
2	A	1782	PGD	C6-C5-N7	-26.15	130.62	134.14
2	C	1783	PGD	C6-C5-N7	-14.69	132.16	134.14
2	A	1783	PGD	C6-C5-N7	-12.23	132.49	134.14
2	A	1782	PGD	C17-C16-N15	8.60	127.00	117.94
2	C	1783	PGD	C4'-O4'-C1'	-7.53	101.57	109.75
2	A	1783	PGD	C4'-O4'-C1'	-5.82	103.42	109.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1782	PGD	C8-N9-C4	-5.41	102.77	106.90
2	C	1783	PGD	C8-N9-C4	-5.18	102.94	106.90
2	C	1782	PGD	O4'-C1'-N9	-4.67	104.10	108.44
2	C	1782	PGD	C23-O11-C11	-4.61	103.01	112.03
2	C	1782	PGD	C17-C16-N15	4.50	122.68	117.94
2	C	1783	PGD	C17-C16-N15	4.41	122.59	117.94
2	C	1783	PGD	N20-C19-N18	-4.35	119.54	126.41
2	C	1783	PGD	N19-C19-N18	4.01	122.36	117.14
2	C	1782	PGD	O4'-C1'-C2'	-3.93	100.75	106.77
2	A	1783	PGD	N20-C19-N18	-3.89	120.27	126.41
2	A	1782	PGD	C21-C16-N15	-3.87	114.20	124.33
2	A	1782	PGD	O11-C23-C14	3.55	113.56	108.67
2	C	1783	PGD	O4'-C1'-C2'	-3.51	101.40	106.77
2	C	1782	PGD	C4'-O4'-C1'	-3.46	105.99	109.75
2	C	1783	PGD	N2-C2-N1	3.45	121.66	117.86
2	A	1783	PGD	O11-C23-N22	-3.45	104.72	109.22
2	A	1783	PGD	O4'-C1'-N9	-3.19	105.47	108.44
2	C	1782	PGD	C5-C4-N9	3.10	111.64	107.16
2	A	1782	PGD	N20-C19-N18	-3.08	121.54	126.41
2	C	1782	PGD	N19-C19-N20	3.07	120.47	116.49
2	C	1782	PGD	N20-C19-N18	-3.04	121.62	126.41
2	C	1782	PGD	C5-C4-N3	-2.86	121.79	125.94
2	A	1783	PGD	O4'-C1'-C2'	-2.81	102.47	106.77
2	C	1783	PGD	C5-C4-N9	2.76	111.16	107.16
2	A	1782	PGD	C4'-O4'-C1'	-2.76	106.75	109.75
2	A	1782	PGD	N19-C19-N18	2.75	120.72	117.14
2	A	1782	PGD	C8-N9-C4	-2.73	104.81	106.90
2	A	1783	PGD	C4-C5-N7	-2.73	107.19	109.52
2	A	1783	PGD	O3A-C10-C11	-2.70	101.53	108.53
2	A	1782	PGD	O4'-C1'-N9	-2.69	105.94	108.44
2	A	1783	PGD	C8-N9-C4	-2.53	104.97	106.90
2	A	1782	PGD	O4'-C1'-C2'	-2.52	102.91	106.77
2	A	1783	PGD	C5-C4-N9	2.50	110.78	107.16
2	A	1782	PGD	C5-C4-N3	-2.46	122.38	125.94
2	A	1782	PGD	C23-O11-C11	-2.40	107.33	112.03
2	A	1783	PGD	N19-C19-N18	2.39	120.25	117.14
2	C	1782	PGD	C21-C16-N15	-2.37	118.12	124.33
2	A	1783	PGD	C17-C16-N15	2.33	120.39	117.94
2	A	1783	PGD	N19-C19-N20	2.31	119.48	116.49
2	C	1783	PGD	C23-O11-C11	2.22	116.38	112.03
2	C	1783	PGD	C2-N3-C4	2.21	118.20	115.09
2	C	1783	PGD	PA-O3A-C10	-2.20	106.20	122.03

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1783	PGD	PA-O3A-C10	-2.15	106.56	122.03
2	A	1782	PGD	C2-N3-C4	2.14	118.10	115.09
2	C	1783	PGD	N2-C2-N3	-2.10	117.45	120.30
2	C	1783	PGD	O3A-C10-C11	-2.09	103.11	108.53
2	C	1782	PGD	C23-N22-C21	2.08	125.18	120.63
2	A	1782	PGD	O17-C17-N18	-2.05	116.80	120.25
2	A	1783	PGD	O11-C11-C12	2.01	114.78	109.81
2	C	1783	PGD	C5-C4-N3	-2.01	123.03	125.94

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.