



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:57 AM UTC

PDB ID : 2W19 / pdb_00002w19
Title : Non-covalent complex between dahp synthase and chorismate mutase from Mycobacterium tuberculosis
Authors : Okvist, M.; Sasso, S.; Roderer, K.; Gamper, M.; Codoni, G.; Krengel, U.; Kast, P.
Deposited on : 2008-10-16
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

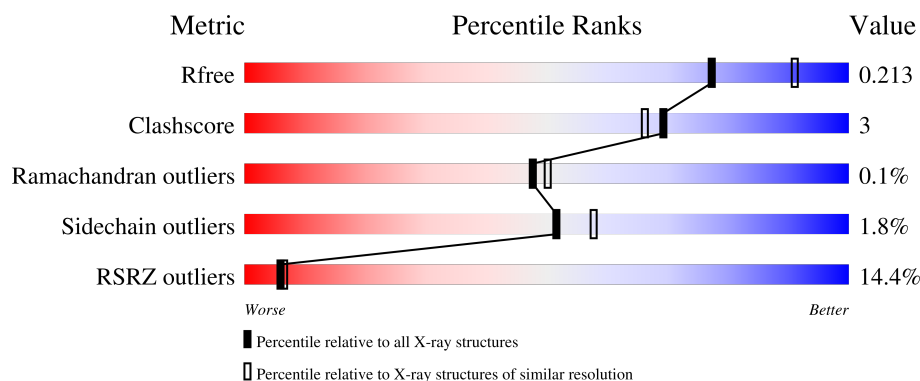
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	472	14% 82% 7% • 11%
1	B	472	9% 79% 9% 12%
2	C	90	20% 76% • 20%
2	D	90	19% 81% • 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1463	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7951 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

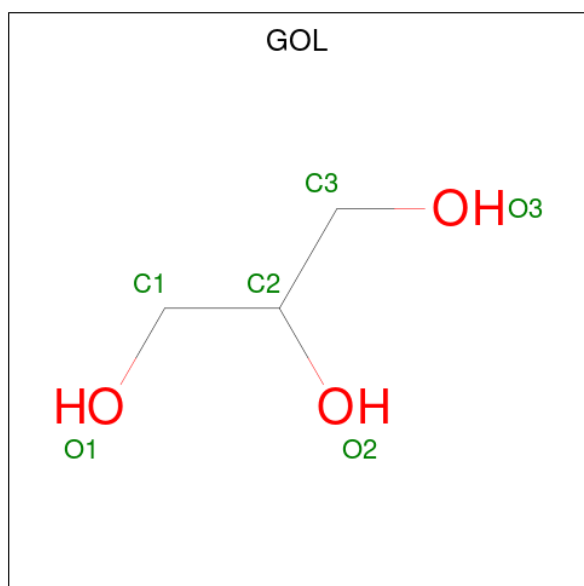
- Molecule 1 is a protein called 3-DEOXY-D-ARABINO-HEPTULOSONATE 7-PHOSPHATE SYNTHASE AROG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	1
			3211	2017	587	592	15			
1	B	417	Total	C	N	O	S	0	0	1
			3189	2001	583	590	15			

- Molecule 2 is a protein called CHORISMATE MUTASE.

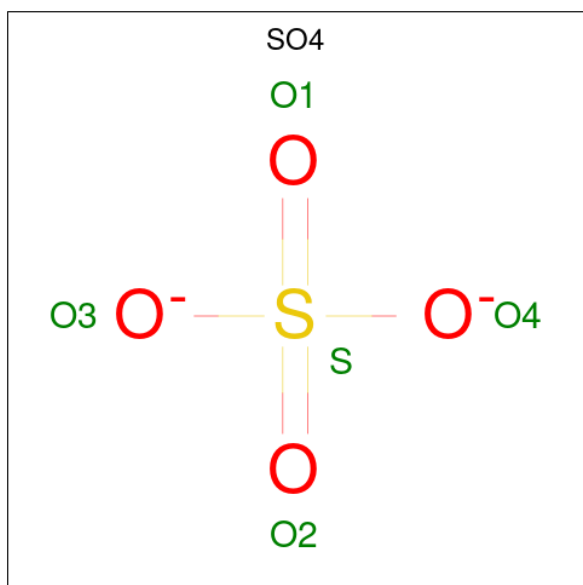
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	72	Total	C	N	O	S	0	0	0
			543	338	108	95	2			
2	D	75	Total	C	N	O	S	0	0	0
			576	357	114	103	2			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

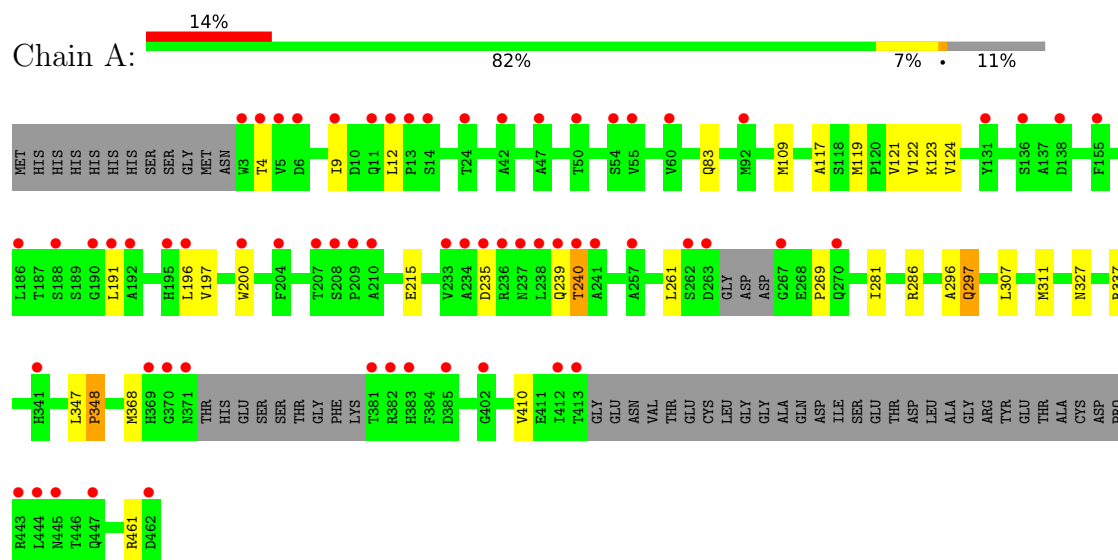
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total	O	0	0
			158	158		
5	B	189	Total	O	0	0
			189	189		
5	C	1	Total	O	0	0
			1	1		
5	D	3	Total	O	0	0
			3	3		

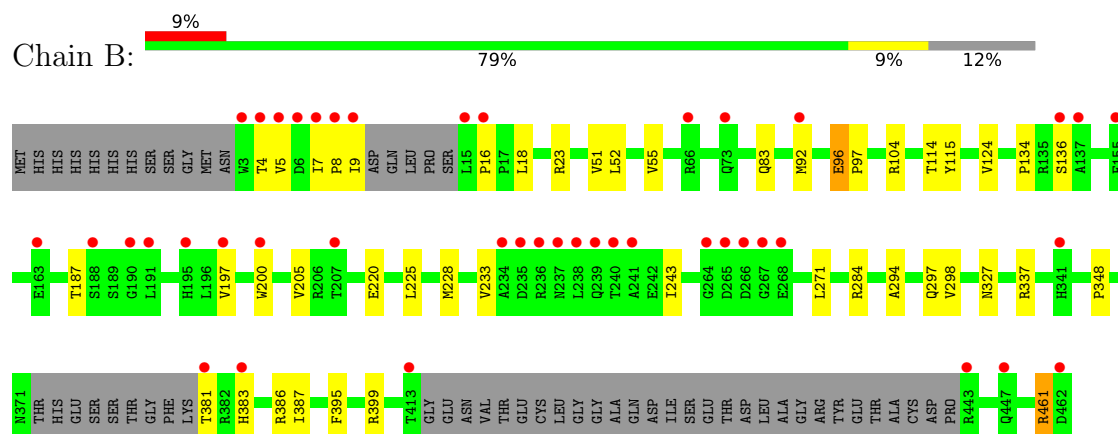
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

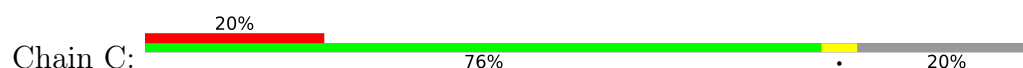
- Molecule 1: 3-DEOXY-D-ARABINO-HEPTULOSONATE 7-PHOSPHATE SYNTHASE AROG



- Molecule 1: 3-DEOXY-D-ARABINO-HEPTULOSONATE 7-PHOSPHATE SYNTHASE AROG

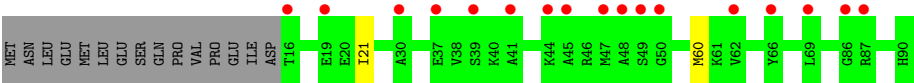
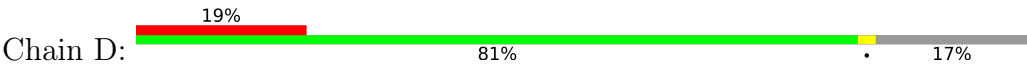


- Molecule 2: CHORISMATE MUTASE





● Molecule 2: CHORISMATE MUTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.02Å 204.02Å 66.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.82 – 2.15 66.82 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.6 (66.82-2.15) 92.5 (66.82-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.211 0.182 , 0.213	Depositor DCC
R_{free} test set	4007 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7951	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, 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	1/3276 (0.0%)	0.82	1/4459 (0.0%)
1	B	0.71	2/3253 (0.1%)	0.81	1/4427 (0.0%)
2	C	0.57	0/546	0.91	0/726
2	D	0.55	0/579	0.86	0/770
All	All	0.67	3/7654 (0.0%)	0.82	2/10382 (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
2	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	PRO	CA-C	7.71	1.56	1.51
1	B	461	ARG	C-N	-5.64	1.25	1.33
1	A	461	ARG	C-N	-5.55	1.25	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	PRO	N-CA-C	5.63	117.58	110.70
1	A	348	PRO	N-CA-C	5.61	117.54	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	20	GLU	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3211	0	3191	24	0
1	B	3189	0	3159	31	0
2	C	543	0	577	1	0
2	D	576	0	614	1	0
3	A	30	0	40	4	0
3	B	36	0	48	4	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	158	0	0	2	0
5	B	189	0	0	2	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
All	All	7951	0	7629	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:HB3	1:A:240:THR:C	1.90	0.95
1:B:197:VAL:HA	1:B:200:TRP:CE3	2.25	0.70
1:A:239:GLN:HB3	1:A:240:THR:CA	2.25	0.66
1:A:197:VAL:HA	1:A:200:TRP:CE3	2.32	0.64
1:B:96:GLU:HG3	1:B:97:PRO:HD3	1.83	0.61
1:B:197:VAL:HA	1:B:200:TRP:CZ3	2.36	0.60
1:A:122:VAL:HA	3:A:1463:GOL:H11	1.83	0.60
1:A:281:ILE:HD11	1:A:296:ALA:HB2	1.85	0.57
1:A:307:LEU:HD22	1:A:311:MET:HE3	1.86	0.56
1:B:9:ILE:HD13	1:B:51:VAL:CG2	2.37	0.55
1:B:297:GLN:NE2	5:B:2135:HOH:O	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD11	1:A:269:PRO:HB3	1.89	0.52
1:B:9:ILE:HD13	1:B:51:VAL:HG23	1.90	0.51
1:A:12:LEU:HD22	1:B:92:MET:HA	1.93	0.51
1:B:9:ILE:CD1	1:B:51:VAL:HG23	2.40	0.51
1:A:4:THR:HG22	1:B:8:PRO:HA	1.93	0.50
1:B:83:GLN:HA	1:B:124:VAL:O	2.13	0.48
1:A:197:VAL:HA	1:A:200:TRP:CZ3	2.48	0.48
1:B:228:MET:HE2	1:B:233:VAL:HG11	1.96	0.47
1:B:395:PHE:O	1:B:399:ARG:HG2	2.16	0.46
1:B:104:ARG:HG3	1:B:200:TRP:CE3	2.52	0.45
1:B:115:TYR:OH	1:B:220:GLU:HG2	2.17	0.45
1:B:294:ALA:HA	1:B:297:GLN:HE21	1.81	0.44
1:B:18:LEU:N	3:B:1469:GOL:H2	2.32	0.44
1:B:381:THR:HG22	1:B:386:ARG:HG3	1.99	0.44
1:A:286:ARG:CZ	1:A:311:MET:HE1	2.48	0.44
1:B:23:ARG:HG2	3:B:1469:GOL:H11	2.00	0.44
1:A:109:MET:HE1	1:A:410:VAL:HG21	1.99	0.44
1:A:121:VAL:O	3:A:1463:GOL:H11	2.18	0.44
1:B:114:THR:OG1	3:B:1464:GOL:H12	2.17	0.44
1:B:271:LEU:HD12	1:B:298:VAL:CG1	2.48	0.44
1:B:134:PRO:HB2	1:B:284:ARG:HD2	2.00	0.43
1:A:123:LYS:NZ	3:A:1463:GOL:H12	2.33	0.43
1:B:104:ARG:HG3	1:B:200:TRP:CZ3	2.53	0.43
1:A:117:ALA:HB1	1:A:119:MET:HG2	2.01	0.43
1:B:383:HIS:CE1	1:B:387:ILE:HD11	2.53	0.43
1:A:297:GLN:NE2	5:A:2133:HOH:O	2.51	0.43
1:B:52:LEU:O	1:B:55:VAL:HG22	2.19	0.42
1:B:197:VAL:HG22	1:B:200:TRP:HZ3	1.84	0.42
1:B:7:ILE:HA	1:B:8:PRO:HD3	1.92	0.42
1:A:327:ASN:ND2	5:A:2141:HOH:O	2.52	0.42
1:A:239:GLN:CB	1:A:240:THR:CA	2.95	0.42
1:B:136:SER:H	3:B:1468:GOL:HO2	1.62	0.42
1:A:83:GLN:HA	1:A:124:VAL:O	2.19	0.42
1:A:4:THR:HG22	1:B:8:PRO:CA	2.50	0.41
2:C:56:HIS:CE1	2:C:60:MET:HE3	2.55	0.41
2:D:60:MET:HE3	2:D:60:MET:HA	2.02	0.41
1:A:9:ILE:HD11	1:B:5:VAL:HG23	2.03	0.41
1:B:327:ASN:ND2	5:B:2151:HOH:O	2.53	0.41
1:A:123:LYS:HZ3	3:A:1463:GOL:C1	2.34	0.41
1:A:368:MET:HE3	1:A:368:MET:HB3	1.93	0.40
1:B:187:THR:CG2	1:B:243:ILE:HD12	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:N	1:A:348:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	411/472 (87%)	403 (98%)	8 (2%)	0	100	100
1	B	409/472 (87%)	403 (98%)	5 (1%)	1 (0%)	43	44
2	C	70/90 (78%)	69 (99%)	1 (1%)	0	100	100
2	D	73/90 (81%)	71 (97%)	2 (3%)	0	100	100
All	All	963/1124 (86%)	946 (98%)	16 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	461	ARG

5.3.2 Protein sidechains [i](#)

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	336/385 (87%)	329 (98%)	7 (2%)	47	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	332/385 (86%)	327 (98%)	5 (2%)	57	64
2	C	53/75 (71%)	52 (98%)	1 (2%)	50	56
2	D	58/75 (77%)	57 (98%)	1 (2%)	53	60
All	All	779/920 (85%)	765 (98%)	14 (2%)	51	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	196	LEU
1	A	215	GLU
1	A	235	ASP
1	A	240	THR
1	A	297	GLN
1	A	337	ARG
1	B	4	THR
1	B	96	GLU
1	B	205	VAL
1	B	225	LEU
1	B	337	ARG
2	C	55	VAL
2	D	21	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	327	ASN
1	B	237	ASN
1	B	297	GLN
1	B	326	HIS
1	B	327	ASN
1	B	383	HIS
2	C	56	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	GOL	B	1464	-	5,5,5	0.40	0	5,5,5	0.37	0
3	GOL	B	1467	-	5,5,5	0.32	0	5,5,5	0.50	0
4	SO4	A	1467	-	4,4,4	0.28	0	6,6,6	0.26	0
3	GOL	B	1465	-	5,5,5	0.32	0	5,5,5	0.29	0
3	GOL	A	1464	-	5,5,5	0.40	0	5,5,5	0.75	0
4	SO4	B	1462	-	4,4,4	0.27	0	6,6,6	0.44	0
3	GOL	B	1468	-	5,5,5	0.60	0	5,5,5	0.45	0
3	GOL	A	1462	-	5,5,5	0.34	0	5,5,5	0.67	0
3	GOL	A	1466	-	5,5,5	0.55	0	5,5,5	0.55	0
3	GOL	A	1465	-	5,5,5	0.40	0	5,5,5	0.21	0
3	GOL	B	1466	-	5,5,5	0.49	0	5,5,5	0.77	0
4	SO4	B	1463	-	4,4,4	0.19	0	6,6,6	0.41	0
3	GOL	A	1463	-	5,5,5	0.77	0	5,5,5	1.33	1 (20%)
3	GOL	B	1469	-	5,5,5	0.93	0	5,5,5	1.42	1 (20%)

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	GOL	B	1464	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1467	-	-	2/4/4/4	-
3	GOL	B	1465	-	-	0/4/4/4	-
3	GOL	A	1464	-	-	2/4/4/4	-
3	GOL	B	1468	-	-	2/4/4/4	-
3	GOL	A	1462	-	-	2/4/4/4	-
3	GOL	A	1466	-	-	3/4/4/4	-
3	GOL	A	1465	-	-	2/4/4/4	-
3	GOL	B	1466	-	-	0/4/4/4	-
3	GOL	A	1463	-	-	3/4/4/4	-
3	GOL	B	1469	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1463	GOL	O1-C1-C2	2.49	121.59	110.38
3	B	1469	GOL	O2-C2-C3	-2.12	100.41	109.18

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1463	GOL	C1-C2-C3-O3
3	A	1465	GOL	C1-C2-C3-O3
3	A	1465	GOL	O2-C2-C3-O3
3	A	1466	GOL	O1-C1-C2-C3
3	B	1468	GOL	O1-C1-C2-C3
3	B	1469	GOL	O1-C1-C2-C3
3	B	1469	GOL	C1-C2-C3-O3
3	B	1467	GOL	O2-C2-C3-O3
3	A	1462	GOL	O1-C1-C2-C3
3	A	1464	GOL	C1-C2-C3-O3
3	B	1467	GOL	C1-C2-C3-O3
3	A	1463	GOL	O2-C2-C3-O3
3	B	1468	GOL	O1-C1-C2-O2
3	B	1469	GOL	O1-C1-C2-O2
3	B	1469	GOL	O2-C2-C3-O3
3	A	1466	GOL	O1-C1-C2-O2
3	A	1462	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1464	GOL	O2-C2-C3-O3
3	A	1463	GOL	O1-C1-C2-O2
3	A	1466	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1464	GOL	1	0
3	B	1468	GOL	1	0
3	A	1463	GOL	4	0
3	B	1469	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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 ²)	Q<0.9
1	A	419/472 (88%)	1.03	64 (15%) 5 5	18, 28, 44, 57	0
1	B	417/472 (88%)	0.58	43 (10%) 12 13	19, 27, 44, 58	0
2	C	72/90 (80%)	1.48	18 (25%) 2 2	23, 32, 35, 36	0
2	D	75/90 (83%)	1.45	17 (22%) 2 2	23, 32, 35, 37	0
All	All	983/1124 (87%)	0.91	142 (14%) 6 6	18, 28, 43, 58	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	ASP	6.3
1	A	191	LEU	5.8
1	A	240	THR	5.8
1	A	3	TRP	5.8
1	B	8	PRO	5.6
2	D	16	THR	5.4
1	A	11	GLN	5.4
1	B	3	TRP	5.1
1	B	6	ASP	5.1
1	B	237	ASN	4.8
1	A	370	GLY	4.6
1	B	191	LEU	4.6
1	B	9	ILE	4.6
1	A	241	ALA	4.6
1	B	462	ASP	4.5
1	A	383	HIS	4.5
1	B	264	GLY	4.5
1	A	13	PRO	4.5
1	A	5	VAL	4.4
1	A	237	ASN	4.4
1	B	7	ILE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	381	THR	4.3
1	B	5	VAL	4.3
1	B	200	TRP	4.3
2	D	50	GLY	4.1
1	B	239	GLN	4.0
1	A	14	SER	3.9
1	A	136	SER	3.8
1	A	54	SER	3.8
1	B	15	LEU	3.7
1	A	4	THR	3.7
1	A	341	HIS	3.7
1	A	190	GLY	3.6
1	B	190	GLY	3.6
1	A	239	GLN	3.6
1	A	235	ASP	3.6
1	A	413	THR	3.6
1	A	236	ARG	3.5
2	C	19	GLU	3.5
1	B	155	PHE	3.4
1	A	369	HIS	3.3
1	B	136	SER	3.3
1	A	412	ILE	3.3
2	C	45	ALA	3.3
1	B	238	LEU	3.3
2	D	41	ALA	3.3
1	A	267	GLY	3.2
1	B	207	THR	3.2
1	A	155	PHE	3.2
1	A	200	TRP	3.1
2	C	21	ILE	3.1
1	A	443	ARG	3.1
1	B	265	ASP	3.1
1	A	92	MET	3.1
1	B	267	GLY	3.1
1	A	402	GLY	3.1
1	A	6	ASP	3.1
1	B	16	PRO	3.0
1	A	234	ALA	3.0
1	A	238	LEU	3.0
1	B	236	ARG	3.0
1	A	12	LEU	3.0
1	B	413	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	22	ASP	3.0
1	B	383	HIS	2.9
1	B	92	MET	2.9
1	B	137	ALA	2.9
2	C	23	ARG	2.8
2	D	30	ALA	2.8
1	A	55	VAL	2.8
1	B	443	ARG	2.8
1	B	235	ASP	2.8
1	B	447	GLN	2.7
1	B	234	ALA	2.7
1	A	188	SER	2.7
2	C	60	MET	2.7
2	D	19	GLU	2.7
2	D	49	SER	2.7
1	A	371	ASN	2.7
2	C	86	GLY	2.7
1	A	210	ALA	2.6
1	B	4	THR	2.6
2	D	86	GLY	2.6
1	A	192	ALA	2.6
1	B	381	THR	2.6
2	C	69	LEU	2.6
1	B	268	GLU	2.5
1	A	204	PHE	2.5
1	A	50	THR	2.5
1	A	209	PRO	2.5
2	D	47	MET	2.5
2	D	87	ARG	2.5
2	C	63	ILE	2.5
1	A	263	ASP	2.4
2	D	45	ALA	2.4
2	C	84	GLY	2.4
1	B	266	ASP	2.4
1	A	207	THR	2.4
1	B	240	THR	2.4
1	B	241	ALA	2.4
2	C	90	HIS	2.4
1	B	73	GLN	2.4
1	A	385	ASP	2.4
1	A	138	ASP	2.4
1	A	9	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	195	HIS	2.4
1	A	196	LEU	2.3
1	A	447	GLN	2.3
1	A	47	ALA	2.3
2	D	44	LYS	2.3
2	C	47	MET	2.3
1	A	382	ARG	2.3
2	C	54	LEU	2.3
1	A	131	TYR	2.3
1	B	197	VAL	2.2
1	A	42	ALA	2.2
2	C	89	GLY	2.2
2	D	66	TYR	2.2
1	B	341	HIS	2.2
2	D	39	SER	2.2
2	D	62	VAL	2.2
2	D	48	ALA	2.2
2	D	69	LEU	2.2
1	B	66	ARG	2.2
2	D	37	GLU	2.1
2	C	48	ALA	2.1
1	B	163	GLU	2.1
1	A	24	THR	2.1
1	A	60	VAL	2.1
1	A	208	SER	2.1
1	B	188	SER	2.1
2	C	39	SER	2.1
1	A	233	VAL	2.1
1	A	444	LEU	2.1
1	A	270	GLN	2.1
1	B	195	HIS	2.1
2	C	58	ARG	2.1
1	A	257	ALA	2.1
2	C	26	ALA	2.1
1	A	186	LEU	2.0
1	A	445	ASN	2.0
1	A	262	SER	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1466	6/6	0.79	0.20	42,48,49,49	0
3	GOL	A	1465	6/6	0.80	0.23	57,60,62,62	0
3	GOL	B	1468	6/6	0.83	0.22	50,52,52,54	0
3	GOL	A	1464	6/6	0.86	0.17	33,41,44,45	0
3	GOL	A	1463	6/6	0.87	0.15	23,29,32,34	0
3	GOL	B	1469	6/6	0.88	0.21	27,32,32,33	0
3	GOL	B	1464	6/6	0.89	0.15	28,30,31,31	0
3	GOL	B	1466	6/6	0.92	0.15	26,33,35,35	0
3	GOL	A	1462	6/6	0.93	0.09	30,31,31,32	0
3	GOL	B	1465	6/6	0.95	0.12	23,25,27,28	0
3	GOL	B	1467	6/6	0.96	0.15	25,29,30,30	0
4	SO4	A	1467	5/5	0.97	0.13	32,35,36,36	0
4	SO4	B	1462	5/5	0.98	0.12	27,28,30,30	0
4	SO4	B	1463	5/5	0.99	0.15	31,31,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.