



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:06 PM UTC

PDB ID : 3VFL / pdb_00003vfl
Title : Structure, Function, Stability and Knockout Phenotype of Dihydrodipicolinate Synthase from *Streptococcus pneumoniae*
Authors : Gorman, M.A.
Deposited on : 2012-01-10
Resolution : 1.91 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

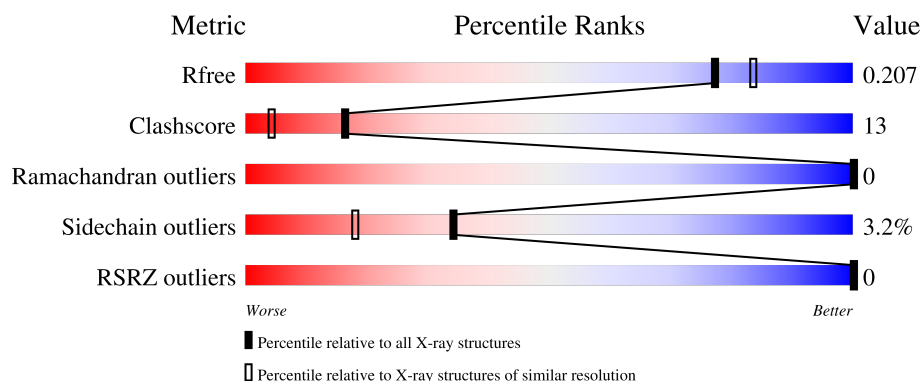
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	311	
1	B	311	

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	403	-	-	X	-
3	GOL	A	405	-	X	X	-
3	GOL	B	403	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5014 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.

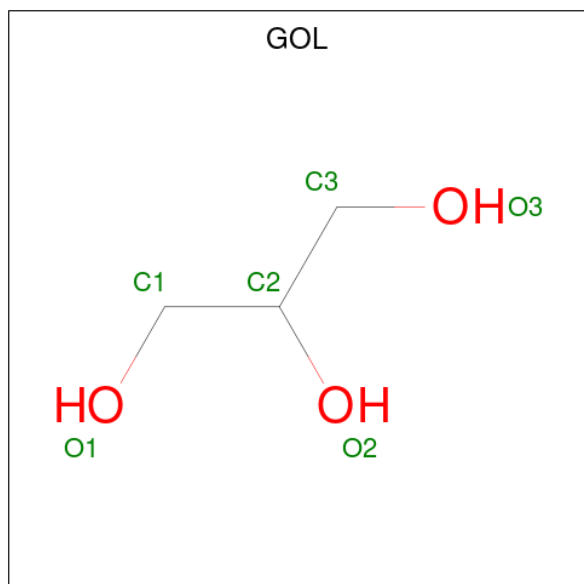
- Molecule 1 is a protein called Dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2366	1516	385	455	10			
1	B	306	Total	C	N	O	S	0	1	0
			2359	1512	383	454	10			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

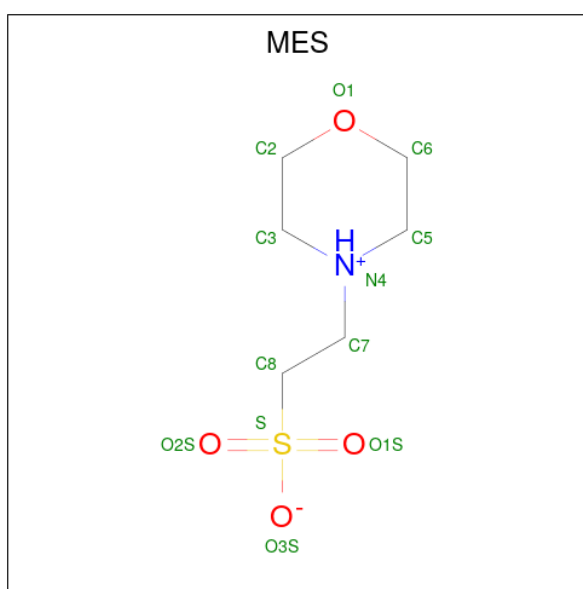
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	B	2	Total	K	0	0
			2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

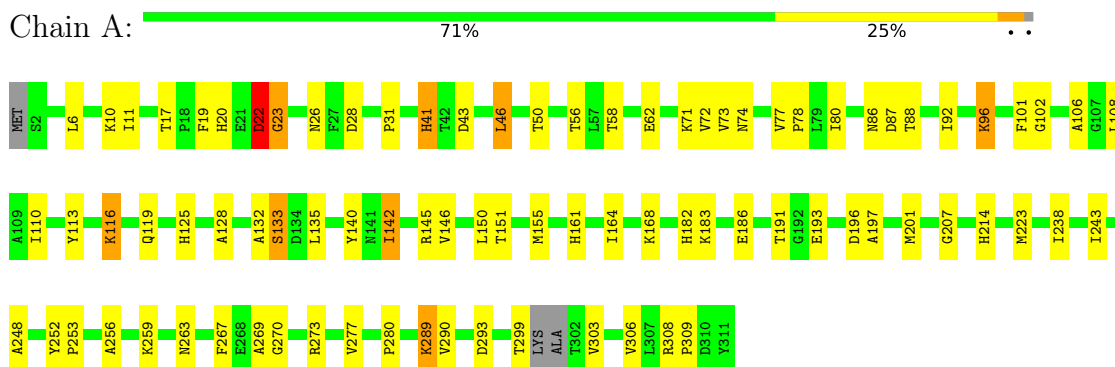
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	118	Total	O	0	0
			118	118		

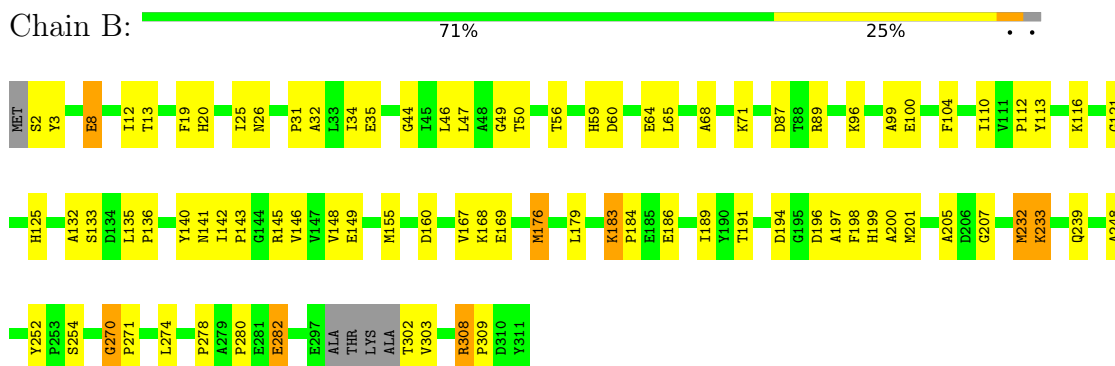
3 Residue-property plots [i](#)

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: Dihydrodipicolinate synthase



- Molecule 1: Dihydrodipicolinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	62.36Å 105.33Å 105.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 1.91 47.83 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.83-1.91) 99.3 (47.83-1.92)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.212 0.165 , 0.207	Depositor DCC
R_{free} test set	2747 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.459 for -h,l,k	Xtriage
Reported twinning fraction	0.541 for H, K, L 0.459 for -H, L, K	Depositor
Outliers	0 of 54037 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5014	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MES, GOL

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	1.38	8/2420 (0.3%)	1.47	28/3293 (0.9%)
1	B	1.41	17/2416 (0.7%)	1.40	15/3287 (0.5%)
All	All	1.40	25/4836 (0.5%)	1.44	43/6580 (0.7%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	LYS	N-CA	10.04	1.53	1.46
1	A	256	ALA	CA-C	8.84	1.61	1.52
1	A	116	LYS	CA-CB	7.92	1.58	1.52
1	B	254	SER	CA-C	6.99	1.60	1.53
1	B	199	HIS	CG-ND1	-6.98	1.30	1.38
1	B	199	HIS	CG-CD2	6.81	1.43	1.35
1	B	148	VAL	CA-C	-6.38	1.44	1.52
1	B	125	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	248	ALA	C-O	5.95	1.31	1.24
1	B	274	LEU	CA-C	5.93	1.59	1.53
1	B	59	HIS	CG-CD2	5.89	1.42	1.35
1	A	125	HIS	CG-CD2	5.54	1.42	1.35
1	B	141	ASN	CA-CB	-5.33	1.45	1.53
1	B	125	HIS	CG-ND1	-5.17	1.32	1.38
1	A	207	GLY	N-CA	-5.13	1.40	1.45
1	A	17	THR	C-O	-5.13	1.19	1.24
1	A	248	ALA	C-O	5.09	1.30	1.24
1	B	59	HIS	CE1-NE2	5.07	1.37	1.32
1	A	243	ILE	CA-CB	5.07	1.56	1.54
1	B	169	GLU	N-CA	-5.07	1.40	1.46
1	B	189	ILE	C-O	-5.04	1.18	1.24
1	B	194	ASP	N-CA	5.03	1.52	1.46
1	B	13	THR	C-O	5.03	1.29	1.23
1	A	183	LYS	CA-C	5.01	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	PHE	CA-C	-5.01	1.46	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	LEU	CA-C-N	-8.90	111.59	120.31
1	B	135	LEU	C-N-CA	-8.90	111.59	120.31
1	B	233	LYS	N-CA-C	-7.54	103.07	111.82
1	B	252	TYR	N-CA-C	-7.48	96.88	108.55
1	A	96	LYS	N-CA-C	-7.23	103.48	111.36
1	B	270	GLY	CA-C-N	-7.12	110.94	119.84
1	B	270	GLY	C-N-CA	-7.12	110.94	119.84
1	A	77	VAL	CA-C-N	-7.00	113.10	120.03
1	A	77	VAL	C-N-CA	-7.00	113.10	120.03
1	A	196	ASP	CB-CA-C	-6.91	97.63	109.65
1	A	183	LYS	CA-C-N	-6.87	113.63	120.98
1	A	183	LYS	C-N-CA	-6.87	113.63	120.98
1	A	23	GLY	N-CA-C	-6.67	105.97	114.37
1	A	135	LEU	CA-C-N	-6.65	113.83	120.21
1	A	135	LEU	C-N-CA	-6.65	113.83	120.21
1	A	22	ASP	N-CA-CB	-6.57	100.19	110.44
1	B	252	TYR	CA-C-N	-6.56	113.01	119.90
1	B	252	TYR	C-N-CA	-6.56	113.01	119.90
1	A	73	VAL	N-CA-C	-6.47	103.88	113.39
1	A	243	ILE	CA-C-N	-6.37	112.28	119.28
1	A	243	ILE	C-N-CA	-6.37	112.28	119.28
1	B	183	LYS	CA-C-N	-6.16	112.14	119.84
1	B	183	LYS	C-N-CA	-6.16	112.14	119.84
1	B	34	ILE	N-CA-C	6.14	116.89	110.62
1	A	243	ILE	N-CA-CB	5.72	114.35	110.52
1	B	71	LYS	N-CA-C	-5.65	105.04	111.14
1	A	11	ILE	CB-CA-C	5.63	116.92	111.23
1	A	290	VAL	N-CA-C	5.57	115.77	110.42
1	A	201	MET	N-CA-C	5.38	117.15	111.28
1	B	232	MET	N-CA-C	5.25	117.01	111.28
1	B	160	ASP	N-CA-C	5.23	118.92	112.54
1	A	17	THR	CA-C-N	-5.23	114.38	119.76
1	A	17	THR	C-N-CA	-5.23	114.38	119.76
1	A	132	ALA	N-CA-C	5.20	118.89	112.54
1	A	214	HIS	CA-C-N	-5.18	114.06	121.98
1	A	214	HIS	C-N-CA	-5.18	114.06	121.98
1	A	102	GLY	N-CA-C	5.18	120.47	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	PHE	N-CA-C	-5.17	105.54	111.07
1	A	71	LYS	N-CA-C	-5.10	105.41	110.97
1	A	86	ASN	N-CA-C	-5.09	106.91	113.02
1	A	267	PHE	N-CA-C	5.08	119.46	113.16
1	A	41	HIS	N-CA-C	5.03	118.72	112.58
1	B	68	ALA	N-CA-C	-5.02	105.50	110.97

There are no chirality outliers.

There are no planarity outliers.

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	2366	0	2336	59	0
1	B	2359	0	2328	68	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	18	0	24	17	0
3	B	6	0	8	17	0
4	A	12	0	13	1	0
4	B	12	0	13	1	0
5	A	119	0	0	4	0
5	B	118	0	0	6	0
All	All	5014	0	4722	123	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 13.

All (123) 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:B:49:GLY:CA	3:B:403:GOL:H31	1.83	1.07
1:B:50:THR:H	3:B:403:GOL:C3	1.67	1.07
1:B:50:THR:H	3:B:403:GOL:H32	1.19	1.02
1:B:50:THR:N	3:B:403:GOL:H32	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:GLY:HA2	3:B:403:GOL:H31	1.48	0.96
1:A:308:ARG:NH1	1:B:89:ARG:HG2	1.92	0.84
1:B:50:THR:N	3:B:403:GOL:C3	2.36	0.83
1:B:176:MET:HE2	1:B:200:ALA:HB1	1.65	0.77
1:A:168:LYS:NZ	3:A:403:GOL:H2	1.99	0.77
1:A:168:LYS:HZ3	3:A:403:GOL:H2	1.49	0.77
3:A:405:GOL:H2	1:B:89:ARG:HB3	1.68	0.76
1:A:56:THR:HB	3:A:405:GOL:H31	1.68	0.75
1:B:176:MET:HE2	1:B:200:ALA:CB	2.18	0.73
1:B:176:MET:HE3	1:B:205:ALA:HB2	1.71	0.72
1:B:176:MET:CE	1:B:200:ALA:HB1	2.20	0.72
1:B:233:LYS:HG3	5:B:530:HOH:O	1.88	0.72
1:A:168:LYS:NZ	3:A:403:GOL:C2	2.53	0.72
1:A:72:VAL:HG12	1:A:72:VAL:O	1.90	0.70
1:B:96:LYS:HE3	1:B:132:ALA:O	1.90	0.70
3:A:405:GOL:H11	1:B:87:ASP:OD1	1.92	0.70
1:A:20:HIS:C	1:A:22:ASP:H	2.01	0.69
1:A:182:HIS:HD2	5:A:580:HOH:O	1.75	0.68
1:B:282:GLU:H	1:B:282:GLU:CD	2.01	0.68
1:B:302:THR:OG1	1:B:303:VAL:N	2.24	0.68
1:B:49:GLY:HA3	3:B:403:GOL:H12	1.76	0.67
1:A:182:HIS:HE1	5:A:525:HOH:O	1.77	0.66
3:A:405:GOL:H2	1:B:89:ARG:CB	2.25	0.66
1:B:50:THR:H	3:B:403:GOL:C2	2.08	0.65
1:B:278:PRO:O	1:B:303:VAL:HG11	1.98	0.64
1:B:176:MET:CE	1:B:205:ALA:HB2	2.28	0.63
1:A:50:THR:N	3:A:403:GOL:H12	2.14	0.63
1:A:263:ASN:OD1	1:A:269:ALA:N	2.33	0.62
1:B:49:GLY:HA3	3:B:403:GOL:H31	1.75	0.62
1:A:72:VAL:O	1:A:72:VAL:CG1	2.47	0.62
1:A:193:GLU:OE1	4:A:406:MES:H21	2.00	0.62
1:A:58:THR:HG23	1:A:308:ARG:HE	1.65	0.61
1:A:140:TYR:CE1	1:A:168:LYS:HE2	2.37	0.59
1:A:46:LEU:HD22	3:A:403:GOL:O2	2.01	0.59
1:B:143:PRO:HB3	1:B:149:GLU:HB3	1.85	0.58
1:B:8:GLU:OE2	1:B:8:GLU:HA	2.04	0.57
1:A:223:MET:HB2	1:A:238:ILE:HG21	1.87	0.57
1:B:99:ALA:HB2	1:B:133:SER:OG	2.05	0.56
1:A:46:LEU:CD2	3:A:403:GOL:O2	2.53	0.56
3:A:405:GOL:C1	1:B:87:ASP:OD1	2.53	0.56
1:A:168:LYS:HZ2	3:A:403:GOL:C2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:HE22	1:A:150:LEU:HA	1.71	0.55
1:A:56:THR:HB	3:A:405:GOL:H11	1.88	0.54
1:B:110:ILE:HA	1:B:140:TYR:HB3	1.90	0.54
1:A:58:THR:O	1:A:62:GLU:HG3	2.07	0.53
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.72	0.53
1:A:20:HIS:C	1:A:22:ASP:N	2.63	0.53
1:B:271:PRO:HA	5:B:517:HOH:O	2.09	0.53
1:B:49:GLY:CA	3:B:403:GOL:C3	2.74	0.52
1:B:184:PRO:HD3	5:B:562:HOH:O	2.12	0.50
1:B:280:PRO:HA	1:B:303:VAL:HG21	1.93	0.50
1:A:88:THR:O	1:A:92:ILE:HG12	2.12	0.50
1:B:113:TYR:HB3	1:B:146:VAL:HG12	1.94	0.50
1:A:191:THR:HG21	1:A:197:ALA:HA	1.93	0.49
1:A:92:ILE:HD11	1:A:128:ALA:HB1	1.93	0.49
1:B:50:THR:OG1	3:B:403:GOL:H32	2.13	0.49
1:A:41:HIS:HE1	5:A:568:HOH:O	1.94	0.49
1:A:289:LYS:O	1:A:293:ASP:HA	2.13	0.49
1:A:277:VAL:HG13	1:B:121:GLY:HA2	1.94	0.49
1:B:198:PHE:CG	1:B:239:GLN:HG2	2.47	0.49
1:A:80:ILE:HG12	1:A:106:ALA:HB3	1.94	0.49
1:A:74:ASN:CG	1:A:74:ASN:O	2.52	0.48
1:B:198:PHE:CD2	1:B:239:GLN:HG2	2.48	0.48
1:B:49:GLY:C	3:B:403:GOL:H31	2.35	0.48
1:B:142:ILE:HG12	1:B:145:ARG:HB2	1.93	0.48
1:A:58:THR:CG2	1:A:308:ARG:HE	2.25	0.48
1:B:201:MET:SD	1:B:207:GLY:HA2	2.54	0.48
1:A:140:TYR:OH	1:A:142:ILE:HD13	2.14	0.48
1:B:155:MET:HE3	1:B:167:VAL:HG21	1.96	0.48
1:B:308:ARG:NH1	5:B:609:HOH:O	2.42	0.47
1:B:133:SER:HB3	5:B:593:HOH:O	2.13	0.47
1:B:46:LEU:CD2	3:B:403:GOL:H11	2.45	0.47
1:B:60:ASP:O	1:B:64:GLU:HG3	2.15	0.47
1:A:26:ASN:OD1	1:A:28:ASP:HB2	2.15	0.46
1:B:140:TYR:OH	4:B:404:MES:O2S	2.34	0.46
1:A:50:THR:H	3:A:403:GOL:H12	1.80	0.46
1:A:116:LYS:HD3	1:B:145:ARG:HG2	1.97	0.46
1:B:25:ILE:HD13	1:B:65:LEU:HD11	1.98	0.46
1:A:142:ILE:HG12	1:A:145:ARG:HB2	1.99	0.45
1:A:110:ILE:HA	1:A:140:TYR:HB3	1.97	0.45
1:B:191:THR:HG21	1:B:197:ALA:HA	1.98	0.45
1:A:110:ILE:HB	3:A:404:GOL:H11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:O	1:B:146:VAL:HG22	2.17	0.45
1:A:96:LYS:HA	1:A:133:SER:HB2	1.98	0.44
1:A:87:ASP:OD1	1:B:56:THR:HA	2.17	0.44
1:A:161:HIS:HB3	1:A:164:ILE:HG13	2.00	0.44
1:B:140:TYR:CD1	1:B:168:LYS:HD3	2.53	0.44
1:B:3:TYR:CE1	1:B:186:GLU:HA	2.53	0.44
1:B:46:LEU:HD23	3:B:403:GOL:H11	2.00	0.44
1:A:23:GLY:CA	1:A:306:VAL:CG1	2.96	0.44
1:B:12:ILE:HA	1:B:44:GLY:O	2.17	0.44
1:B:3:TYR:CZ	1:B:186:GLU:HA	2.53	0.43
1:B:31:PRO:O	1:B:35:GLU:HG2	2.19	0.43
1:A:19:PHE:O	1:A:270:GLY:HA3	2.19	0.43
1:A:155:MET:HE2	1:A:155:MET:HB2	1.96	0.43
1:A:56:THR:O	3:A:405:GOL:C3	2.66	0.42
1:B:49:GLY:C	3:B:403:GOL:C3	2.90	0.42
1:A:113:TYR:HB3	1:A:146:VAL:HG12	2.02	0.42
1:A:252:TYR:CD2	1:A:253:PRO:HD2	2.54	0.42
1:B:20:HIS:CE1	1:B:26:ASN:HA	2.54	0.42
1:A:140:TYR:CZ	1:A:168:LYS:HE2	2.55	0.41
1:B:19:PHE:O	1:B:270:GLY:HA3	2.20	0.41
1:B:50:THR:N	3:B:403:GOL:H12	2.34	0.41
1:A:43:ASP:O	1:A:78:PRO:HD2	2.19	0.41
1:A:259:LYS:HE3	5:A:511:HOH:O	2.18	0.41
1:B:32:ALA:N	5:B:532:HOH:O	2.41	0.41
1:A:108:LEU:HD21	1:A:140:TYR:HB2	2.02	0.41
1:A:119:GLN:NE2	1:A:151:THR:H	2.18	0.41
1:A:10:LYS:N	1:A:43:ASP:OD2	2.39	0.41
1:B:47:LEU:HA	1:B:47:LEU:HD23	1.85	0.41
1:B:49:GLY:CA	3:B:403:GOL:H12	2.49	0.41
1:A:6:LEU:HA	1:A:6:LEU:HD23	1.78	0.40
1:A:280:PRO:HA	1:A:303:VAL:HG21	2.03	0.40
1:B:179:LEU:O	1:B:183:LYS:HB3	2.22	0.40
1:A:273:ARG:CZ	1:A:308:ARG:HB3	2.51	0.40
3:A:405:GOL:H2	1:B:89:ARG:HB2	2.03	0.40
1:B:2:SER:HA	1:B:136:PRO:HG2	2.04	0.40
1:A:28:ASP:O	1:A:31:PRO:HD2	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	304/311 (98%)	290 (95%)	14 (5%)	0	100	100
1	B	303/311 (97%)	290 (96%)	13 (4%)	0	100	100
All	All	607/622 (98%)	580 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	253/255 (99%)	245 (97%)	8 (3%)	34	18
1	B	253/255 (99%)	245 (97%)	8 (3%)	34	18
All	All	506/510 (99%)	490 (97%)	16 (3%)	34	18

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

Mol	Chain	Res	Type
1	A	22	ASP
1	A	46	LEU
1	A	133	SER
1	A	142	ILE
1	A	186	GLU
1	A	289	LYS
1	A	299	THR
1	A	309	PRO

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Mol	Chain	Res	Type
1	B	8	GLU
1	B	100	GLU
1	B	112	PRO
1	B	176	MET
1	B	232	MET
1	B	282	GLU
1	B	308	ARG
1	B	309	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	41	HIS
1	A	74	ASN
1	A	119	GLN
1	A	182	HIS
1	B	36	HIS
1	B	41	HIS
1	B	182	HIS
1	B	202	ASN
1	B	216	ASN
1	B	221	HIS

5.3.3 RNA [i](#)

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](#)

Of 10 ligands modelled in this entry, 4 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$
4	MES	A	406	-	12,12,12	2.31	1 (8%)	15,16,16	5.59	11 (73%)
3	GOL	A	404	-	5,5,5	0.34	0	5,5,5	1.01	0
3	GOL	B	403	-	5,5,5	0.94	0	5,5,5	1.12	0
3	GOL	A	403	-	5,5,5	0.42	0	5,5,5	0.59	0
3	GOL	A	405	-	5,5,5	0.71	0	5,5,5	1.90	2 (40%)
4	MES	B	404	-	12,12,12	2.68	2 (16%)	15,16,16	5.85	8 (53%)

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
4	MES	A	406	-	-	5/6/14/14	0/1/1/1
3	GOL	A	404	-	-	4/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
3	GOL	A	403	-	-	4/4/4/4	-
3	GOL	A	405	-	-	4/4/4/4	-
4	MES	B	404	-	-	4/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	MES	C8-S	-8.71	1.65	1.77
4	A	406	MES	C8-S	-7.16	1.67	1.77
4	B	404	MES	O2S-S	2.06	1.50	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	MES	O1S-S-C8	12.42	125.50	106.73
4	A	406	MES	O3S-S-O1S	-11.14	83.52	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	MES	O3S-S-O1S	-10.24	85.79	111.40
4	B	404	MES	O3S-S-C8	-9.84	86.76	106.00
4	A	406	MES	O3S-S-O2S	-9.84	86.79	111.40
4	B	404	MES	O3S-S-O2S	-9.50	87.63	111.40
4	A	406	MES	O2S-S-C8	8.07	118.92	106.73
4	A	406	MES	O3S-S-C8	-7.85	90.64	106.00
4	A	406	MES	O1S-S-C8	7.57	118.17	106.73
4	B	404	MES	O2S-S-C8	4.46	113.46	106.73
4	A	406	MES	O1-C2-C3	4.36	121.16	111.77
4	B	404	MES	C6-C5-N4	-4.11	103.87	110.12
4	B	404	MES	C2-C3-N4	-3.64	104.58	110.12
4	A	406	MES	C2-C3-N4	3.37	115.25	110.12
3	A	405	GOL	O2-C2-C1	-3.14	96.20	109.18
4	A	406	MES	C8-C7-N4	2.75	122.76	112.36
4	A	406	MES	O2S-S-O1S	2.53	122.06	113.82
4	A	406	MES	C6-C5-N4	-2.40	106.47	110.12
3	A	405	GOL	C3-C2-C1	-2.29	103.40	111.80
4	A	406	MES	C7-N4-C3	2.26	117.27	111.24
4	B	404	MES	C6-O1-C2	2.23	117.08	109.88

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O1-C1-C2-C3
3	A	404	GOL	C1-C2-C3-O3
3	A	405	GOL	O1-C1-C2-O2
3	A	405	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-C3
4	A	406	MES	C8-C7-N4-C3
4	A	406	MES	C8-C7-N4-C5
4	A	406	MES	N4-C7-C8-S
4	A	406	MES	C7-C8-S-O2S
4	B	404	MES	C8-C7-N4-C3
4	B	404	MES	C7-C8-S-O2S
3	A	405	GOL	O2-C2-C3-O3
4	B	404	MES	C7-C8-S-O3S
3	A	403	GOL	O1-C1-C2-C3
3	A	403	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O2-C2-C3-O3
4	B	404	MES	C8-C7-N4-C5
3	B	403	GOL	O2-C2-C3-O3
3	A	403	GOL	O1-C1-C2-O2
4	A	406	MES	C7-C8-S-O1S
3	B	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	406	MES	1	0
3	A	404	GOL	1	0
3	B	403	GOL	17	0
3	A	403	GOL	8	0
3	A	405	GOL	8	0
4	B	404	MES	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	308/311 (99%)	-1.14	0 100 100	16, 27, 44, 59	0
1	B	306/311 (98%)	-1.12	0 100 100	13, 27, 43, 65	1 (0%)
All	All	614/622 (98%)	-1.13	0 100 100	13, 27, 44, 65	1 (0%)

There are no RSRZ outliers to report.

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

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(Å ²)	Q<0.9
2	K	A	401	1/1	0.98	0.06	44,44,44,44	0
2	K	B	402	1/1	0.98	0.08	48,48,48,48	0
3	GOL	A	404	6/6	0.98	0.08	25,32,38,44	0
3	GOL	A	405	6/6	0.98	0.06	13,15,16,16	6
4	MES	B	404	12/12	0.98	0.05	33,43,49,52	0
2	K	B	401	1/1	0.99	0.04	46,46,46,46	0
2	K	A	402	1/1	0.99	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	403	6/6	0.99	0.08	21,24,28,33	6
4	MES	A	406	12/12	0.99	0.04	28,32,45,46	0
3	GOL	A	403	6/6	0.99	0.10	30,39,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.