



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:59 PM UTC

PDB ID : 3PUE / pdb_00003pue
Title : Crystal structure of the complex of Dhydrodipicolinate synthase from *Acinetobacter baumannii* with lysine at 2.6Å resolution
Authors : Jithesh, O.; Yamini, S.; Kaur, N.; Gautam, A.; Tewari, R.; Kushwaha, G.S.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.
Deposited on : 2010-12-04
Resolution : 2.60 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

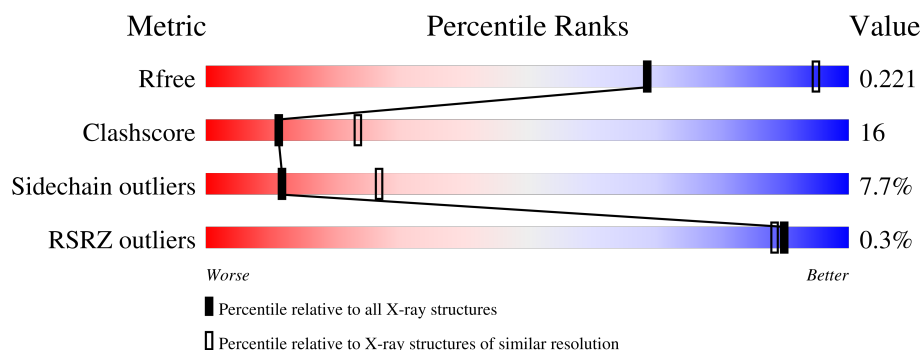
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	291	61% 31% 8%
1	B	291	67% 27% 5%

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	LYS	B	292	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4597 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	291	Total	C	N	O	S	0	0	0
			2195	1387	374	426	8			
1	B	291	Total	C	N	O	S	0	0	0
			2195	1387	374	426	8			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

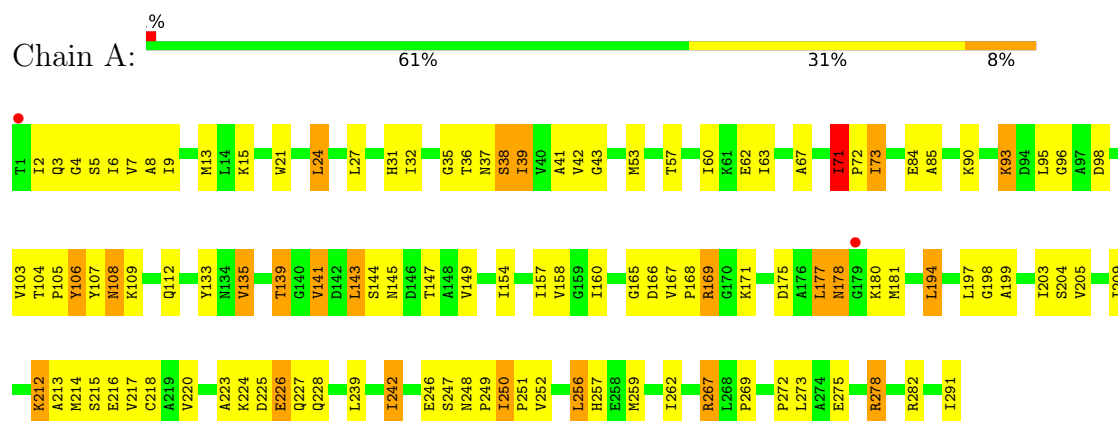
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total 76	O 76	0	0
5	B	88	Total 88	O 88	0	0

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	H 3	Depositor
Cell constants a, b, c, α , β , γ	169.04Å 169.04Å 61.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.80 – 2.60 48.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.80-2.60) 99.7 (48.80-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.235 0.198 , 0.221	Depositor DCC
R_{free} test set	1032 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: SO4, 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	0.69	3/2229 (0.1%)	1.16	25/3033 (0.8%)
1	B	0.69	5/2229 (0.2%)	1.09	17/3033 (0.6%)
All	All	0.69	8/4458 (0.2%)	1.13	42/6066 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	ILE	C-O	-8.58	1.17	1.24
1	B	250	ILE	C-O	-6.74	1.18	1.24
1	B	6	ILE	C-O	-6.43	1.17	1.24
1	A	242	ILE	C-O	-5.96	1.16	1.24
1	A	160	ILE	CA-CB	-5.45	1.47	1.54
1	B	2	ILE	C-O	-5.37	1.18	1.24
1	B	242	ILE	C-O	-5.34	1.17	1.24
1	B	53	MET	SD-CE	5.25	1.92	1.79

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASN	N-CA-C	-14.20	90.56	108.45
1	B	204	SER	N-CA-C	9.53	125.26	110.20
1	A	205	VAL	N-CA-C	-9.13	103.00	111.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	SER	N-CA-C	8.02	123.08	110.32
1	A	135	VAL	CA-C-N	7.64	129.40	119.84
1	A	135	VAL	C-N-CA	7.64	129.40	119.84
1	A	158	VAL	N-CA-C	7.24	120.00	112.83
1	A	43	GLY	N-CA-C	-6.98	103.01	112.57
1	A	139	THR	N-CA-C	6.68	121.66	112.90
1	A	9	ILE	N-CA-C	6.55	118.12	109.21
1	A	2	ILE	N-CA-C	-6.52	98.88	108.54
1	B	11	THR	CA-C-N	6.39	126.42	119.90
1	B	11	THR	C-N-CA	6.39	126.42	119.90
1	A	278	ARG	N-CA-C	6.31	118.68	111.11
1	A	71	ILE	CA-C-N	-6.23	113.55	119.85
1	A	71	ILE	C-N-CA	-6.23	113.55	119.85
1	A	248	ASN	N-CA-C	-6.14	101.84	109.64
1	A	267	ARG	N-CA-C	6.14	120.27	109.96
1	A	246	GLU	N-CA-C	-6.06	100.09	109.24
1	A	177	LEU	N-CA-C	-5.89	100.73	109.86
1	B	156	ASN	N-CA-C	5.63	119.24	112.93
1	A	165	GLY	N-CA-C	-5.63	107.55	115.32
1	B	226	GLU	N-CA-C	5.62	117.41	111.28
1	A	4	GLY	N-CA-C	5.61	121.98	112.22
1	A	8	ALA	N-CA-C	-5.57	97.52	107.98
1	A	282	ARG	N-CA-C	-5.46	104.56	111.11
1	A	71	ILE	N-CA-C	-5.41	104.76	109.19
1	B	205	VAL	N-CA-C	-5.33	105.92	111.58
1	A	24	LEU	N-CA-C	-5.31	105.19	110.97
1	B	43	GLY	N-CA-C	-5.23	103.67	112.77
1	B	203	ILE	N-CA-C	-5.22	100.62	106.21
1	B	135	VAL	CA-C-N	5.20	126.34	119.84
1	B	135	VAL	C-N-CA	5.20	126.34	119.84
1	B	10	VAL	CB-CA-C	-5.19	105.88	111.59
1	B	7	VAL	N-CA-C	5.16	115.70	108.89
1	A	39	ILE	N-CA-C	5.14	116.12	108.46
1	B	248	ASN	N-CA-C	-5.14	103.11	109.64
1	B	188	ASP	N-CA-C	5.10	117.50	111.33
1	A	85	ALA	N-CA-C	-5.07	105.83	111.36
1	B	246	GLU	N-CA-C	-5.02	101.66	109.24
1	B	9	ILE	N-CA-C	5.02	116.85	109.63
1	B	157	ILE	N-CA-C	-5.01	98.92	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	TYR	Sidechain

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	2195	0	2251	77	0
1	B	2195	0	2251	70	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	B	10	0	12	8	0
4	B	18	0	24	4	0
5	A	76	0	0	3	0
5	B	88	0	0	1	0
All	All	4597	0	4538	145	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 16.

All (145) 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:156:ASN:HD22	1:B:156:ASN:H	1.09	0.95
1:A:109:LYS:HZ2	3:B:292:LYS:HD3	1.38	0.88
1:A:71:ILE:H	1:A:71:ILE:HD13	1.42	0.83
1:A:57:THR:HG23	1:A:95:LEU:HD11	1.59	0.83
1:A:109:LYS:NZ	3:B:292:LYS:HD3	1.95	0.81
1:A:5:SER:H	1:A:37:ASN:HD22	1.30	0.79
1:A:71:ILE:HD13	1:A:71:ILE:N	1.98	0.78
1:A:178:ASN:C	1:A:180:LYS:H	1.91	0.78
1:A:178:ASN:O	1:A:180:LYS:N	2.17	0.77
1:A:194:LEU:HD13	1:A:199:ALA:HB2	1.66	0.77
1:B:244:PHE:HD1	3:B:292:LYS:HG2	1.50	0.77
1:B:209:ILE:HG22	1:B:256:LEU:HD13	1.69	0.74
1:A:209:ILE:HG22	1:A:256:LEU:HD13	1.69	0.73
1:B:247:SER:HA	3:B:292:LYS:HD2	1.70	0.72
1:A:250:ILE:HB	1:A:251:PRO:HD3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:O	1:B:124:GLU:HG3	1.91	0.69
1:B:15:LYS:HE2	1:B:263:ASP:OD1	1.93	0.69
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.74	0.69
1:B:214:MET:HE3	1:B:217:VAL:HB	1.75	0.68
1:B:156:ASN:H	1:B:156:ASN:ND2	1.88	0.68
1:A:31:HIS:HD2	1:A:36:THR:OG1	1.76	0.68
1:B:89:THR:HG22	1:B:126:VAL:HG11	1.76	0.67
1:B:156:ASN:HD22	1:B:156:ASN:N	1.86	0.67
1:A:212:LYS:O	1:A:216:GLU:HG3	1.95	0.67
1:A:220:VAL:HG13	1:A:225:ASP:HB3	1.77	0.67
1:A:41:ALA:HB3	1:A:60:ILE:HD13	1.77	0.64
1:A:178:ASN:C	1:A:180:LYS:N	2.53	0.64
1:B:220:VAL:HG11	1:B:228:GLN:HB3	1.79	0.64
1:A:214:MET:HE1	1:A:218:CYS:SG	2.39	0.63
1:B:227:GLN:HG3	4:B:293:GOL:O1	1.99	0.62
1:A:145:ASN:O	1:A:149:VAL:HG23	2.00	0.62
1:A:112:GLN:HE22	1:A:144:SER:H	1.47	0.61
1:A:72:PRO:HA	1:A:98:ASP:OD2	2.01	0.60
1:B:41:ALA:HB3	1:B:60:ILE:HD13	1.81	0.60
1:B:214:MET:HE2	1:B:218:CYS:SG	2.42	0.60
1:B:67:ALA:CB	1:B:73:ILE:HD11	2.33	0.59
1:A:112:GLN:NE2	1:A:147:THR:OG1	2.31	0.59
1:A:141:VAL:HG22	5:A:318:HOH:O	2.02	0.59
1:A:108:ASN:HD22	1:A:108:ASN:H	1.50	0.58
1:A:108:ASN:H	1:A:108:ASN:ND2	2.00	0.58
1:B:261:LEU:CD2	4:B:296:GOL:H2	2.34	0.58
1:A:143:LEU:CD2	1:A:147:THR:HB	2.34	0.58
1:A:167:VAL:HB	1:A:168:PRO:HD3	1.86	0.57
1:B:202:ASN:ND2	1:B:204:SER:HB2	2.20	0.57
1:A:103:VAL:HA	1:A:133:TYR:HB3	1.86	0.57
1:A:38:SER:HB2	1:A:72:PRO:HG2	1.87	0.56
1:A:108:ASN:HD22	1:A:108:ASN:N	2.02	0.56
1:A:135:VAL:O	1:A:135:VAL:HG13	2.06	0.56
1:A:5:SER:N	1:A:37:ASN:HD22	2.00	0.56
1:B:154:ILE:HB	1:B:157:ILE:HD12	1.88	0.56
1:B:138:ARG:HE	3:B:292:LYS:HA	1.70	0.55
1:B:41:ALA:CB	1:B:60:ILE:HD13	2.36	0.55
1:A:71:ILE:N	1:A:71:ILE:CD1	2.68	0.55
1:B:142:ASP:CG	1:B:169:ARG:HH12	2.15	0.55
1:B:277:TYR:O	1:B:280:PRO:HD2	2.06	0.55
1:B:135:VAL:O	1:B:135:VAL:HG13	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:O	1:A:273:LEU:C	2.50	0.55
1:A:109:LYS:HE2	1:B:138:ARG:HG2	1.89	0.55
1:A:213:ALA:O	1:A:217:VAL:HG23	2.07	0.55
1:B:279:GLU:HB3	1:B:280:PRO:HD3	1.89	0.54
1:B:259:MET:HE3	1:B:290:ILE:CG2	2.38	0.54
1:B:286:LYS:HG2	1:B:291:ILE:HG13	1.88	0.54
1:A:171:LYS:HD3	1:A:197:LEU:HD22	1.90	0.54
1:A:67:ALA:HB2	1:A:73:ILE:HD11	1.89	0.53
1:A:41:ALA:CB	1:A:60:ILE:HD13	2.39	0.53
1:A:143:LEU:HD23	1:A:147:THR:HB	1.91	0.53
1:A:154:ILE:HB	1:A:157:ILE:HD12	1.91	0.53
1:A:275:GLU:HA	1:A:278:ARG:HD2	1.91	0.52
1:B:145:ASN:O	1:B:149:VAL:HG23	2.09	0.52
1:A:175:ASP:O	1:A:177:LEU:O	2.27	0.52
1:A:220:VAL:HG11	1:A:228:GLN:HB3	1.92	0.52
1:A:226:GLU:HG3	1:A:227:GLN:N	2.23	0.52
1:B:244:PHE:CD1	3:B:292:LYS:HG2	2.40	0.52
1:B:256:LEU:HB3	1:B:262:ILE:HG12	1.92	0.52
1:B:138:ARG:HE	3:B:292:LYS:CA	2.23	0.52
1:A:166:ASP:CG	1:A:169:ARG:HB3	2.35	0.51
1:B:205:VAL:O	1:B:208:ASN:HB2	2.11	0.51
1:B:250:ILE:HB	1:B:251:PRO:HD3	1.92	0.51
1:B:64:ILE:HA	1:B:73:ILE:HD13	1.93	0.49
1:A:32:ILE:HG12	1:A:71:ILE:HD12	1.95	0.49
1:B:142:ASP:OD2	1:B:169:ARG:NH1	2.46	0.49
1:A:106:TYR:HB3	1:A:139:THR:HG22	1.94	0.49
1:B:138:ARG:NE	3:B:292:LYS:HA	2.28	0.48
1:A:35:GLY:O	1:A:36:THR:C	2.55	0.47
1:A:42:VAL:HG12	1:A:42:VAL:O	2.14	0.47
1:B:42:VAL:O	1:B:48:ALA:HB2	2.14	0.47
1:B:91:ALA:O	1:B:95:LEU:HG	2.14	0.47
1:A:104:THR:O	1:A:105:PRO:C	2.56	0.47
1:B:103:VAL:HA	1:B:133:TYR:HB3	1.95	0.47
1:B:26:LYS:HD2	4:B:296:GOL:H31	1.96	0.47
1:B:41:ALA:HB3	1:B:60:ILE:CD1	2.44	0.47
1:A:257:HIS:C	1:A:259:MET:H	2.23	0.47
1:A:6:ILE:O	1:A:203:ILE:HA	2.15	0.46
1:A:209:ILE:HG22	1:A:256:LEU:CD1	2.42	0.46
1:B:6:ILE:HG23	1:B:38:SER:HB3	1.97	0.46
1:B:211:PRO:O	1:B:215:SER:HB2	2.15	0.46
1:B:227:GLN:O	1:B:231:THR:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:C	1:A:291:ILE:HD12	2.40	0.46
1:A:7:VAL:CG1	1:A:39:ILE:HG12	2.45	0.46
1:B:220:VAL:CG1	1:B:228:GLN:HB3	2.45	0.46
1:A:31:HIS:CD2	1:A:36:THR:OG1	2.64	0.45
1:B:31:HIS:HE1	5:B:335:HOH:O	2.00	0.45
1:A:67:ALA:CB	1:A:73:ILE:CD1	2.94	0.45
1:B:52:SER:HB3	1:B:55:GLU:HB2	1.97	0.45
1:B:133:TYR:CD1	1:B:161:LYS:HD3	2.52	0.45
1:A:5:SER:H	1:A:37:ASN:ND2	2.07	0.44
1:B:47:GLU:OE2	1:B:253:LYS:CE	2.65	0.44
1:B:195:MET:O	1:B:224:LYS:HE2	2.18	0.44
1:B:279:GLU:OE2	1:B:279:GLU:HA	2.17	0.44
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.88	0.44
1:A:214:MET:CE	1:A:218:CYS:SG	3.05	0.43
1:B:227:GLN:CG	4:B:293:GOL:O1	2.63	0.43
1:A:41:ALA:HB1	1:A:63:ILE:HD12	2.01	0.43
1:B:31:HIS:HD2	1:B:36:THR:OG1	2.02	0.43
1:A:198:GLY:O	1:A:199:ALA:C	2.62	0.42
1:B:209:ILE:HD13	1:B:290:ILE:HD13	2.02	0.42
1:B:135:VAL:O	1:B:135:VAL:HG22	2.19	0.42
1:B:276:GLN:H	1:B:276:GLN:HG3	1.50	0.42
1:A:247:SER:HA	5:A:335:HOH:O	2.18	0.42
1:B:277:TYR:C	1:B:280:PRO:HD2	2.45	0.42
1:A:106:TYR:O	1:A:107:TYR:HB3	2.20	0.42
1:A:62:GLU:OE2	1:A:62:GLU:HA	2.20	0.42
1:B:67:ALA:HB2	1:B:73:ILE:HD11	2.02	0.42
1:A:223:ALA:O	1:A:224:LYS:HB2	2.20	0.41
1:B:102:LEU:HD12	1:B:102:LEU:N	2.34	0.41
1:B:239:LEU:HD21	1:B:290:ILE:HD11	2.01	0.41
1:A:67:ALA:HB2	1:A:73:ILE:CD1	2.50	0.41
1:A:269:PRO:HB2	1:B:110:PRO:HB3	2.03	0.41
1:B:72:PRO:HA	1:B:98:ASP:OD2	2.20	0.41
1:A:24:LEU:O	1:A:27:LEU:HB2	2.21	0.41
1:B:259:MET:HE3	1:B:290:ILE:HG23	2.02	0.41
1:A:249:PRO:O	1:A:252:VAL:HG12	2.20	0.41
1:B:40:VAL:HA	1:B:74:ILE:O	2.21	0.41
1:B:47:GLU:OE2	1:B:253:LYS:HE2	2.20	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.94	0.41
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.81	0.41
1:A:13:MET:SD	1:A:267:ARG:HG3	2.61	0.41
1:A:67:ALA:CB	1:A:73:ILE:HD11	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HB2	1:A:90:LYS:HE3	1.91	0.41
1:B:47:GLU:O	1:B:51:LEU:HG	2.20	0.41
1:A:93:LYS:O	1:A:96:GLY:N	2.40	0.40
1:A:171:LYS:HG3	5:A:317:HOH:O	2.21	0.40
1:A:21:TRP:O	1:A:24:LEU:HB3	2.21	0.40
1:B:53:MET:O	1:B:56:HIS:HB3	2.22	0.40
1:B:196:LEU:HD22	1:B:226:GLU:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	234/234 (100%)	214 (92%)	20 (8%)	10	22
1	B	234/234 (100%)	219 (94%)	15 (6%)	16	35
All	All	468/468 (100%)	433 (92%)	35 (8%)	12	28

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	LYS
1	A	38	SER
1	A	53	MET
1	A	71	ILE
1	A	73	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	84	GLU
1	A	93	LYS
1	A	108	ASN
1	A	141	VAL
1	A	143	LEU
1	A	169	ARG
1	A	181	MET
1	A	194	LEU
1	A	212	LYS
1	A	215	SER
1	A	226	GLU
1	A	239	LEU
1	A	242	ILE
1	A	256	LEU
1	B	16	ASP
1	B	53	MET
1	B	55	GLU
1	B	69	LYS
1	B	73	ILE
1	B	105	PRO
1	B	156	ASN
1	B	169	ARG
1	B	194	LEU
1	B	236	ILE
1	B	239	LEU
1	B	242	ILE
1	B	256	LEU
1	B	270	LEU
1	B	276	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	37	ASN
1	A	108	ASN
1	A	112	GLN
1	A	202	ASN
1	A	283	ASN
1	B	31	HIS
1	B	34	GLN
1	B	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	68	ASN
1	B	156	ASN
1	B	202	ASN
1	B	228	GLN
1	B	276	GLN

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](#)

7 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	$\# Z > 2$
4	GOL	B	294	-	5,5,5	0.98	0	5,5,5	0.98	0
2	SO4	A	292	-	4,4,4	0.71	0	6,6,6	0.45	0
4	GOL	B	296	-	5,5,5	0.83	0	5,5,5	0.79	0
2	SO4	B	295	-	4,4,4	0.71	0	6,6,6	0.45	0
2	SO4	A	293	-	4,4,4	0.78	0	6,6,6	0.37	0
3	LYS	B	292	-	8,9,9	1.22	0	7,10,10	0.91	1 (14%)
4	GOL	B	293	-	5,5,5	0.72	0	5,5,5	0.82	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
4	GOL	B	294	-	-	2/4/4/4	-
4	GOL	B	296	-	-	2/4/4/4	-
3	LYS	B	292	-	-	5/9/9/9	-
4	GOL	B	293	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	292	LYS	OXT-C-O	-2.10	119.31	124.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	292	LYS	O-C-CA-N
4	B	293	GOL	C1-C2-C3-O3
4	B	294	GOL	O1-C1-C2-C3
4	B	294	GOL	O1-C1-C2-O2
3	B	292	LYS	OXT-C-CA-N
4	B	296	GOL	O1-C1-C2-C3
4	B	293	GOL	O2-C2-C3-O3
4	B	296	GOL	O1-C1-C2-O2
3	B	292	LYS	CA-CB-CG-CD
3	B	292	LYS	N-CA-CB-CG
3	B	292	LYS	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	296	GOL	2	0
3	B	292	LYS	8	0
4	B	293	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 [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	291/291 (100%)	-0.10	2 (0%) 84 82	22, 38, 50, 55	0
1	B	291/291 (100%)	-0.41	0 100 100	16, 29, 43, 55	0
All	All	582/582 (100%)	-0.26	2 (0%) 90 88	16, 34, 48, 55	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	GLY	2.2
1	A	1	THR	2.2

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
4	GOL	B	294	6/6	0.80	0.17	58,59,60,61	0
4	GOL	B	293	6/6	0.81	0.13	54,58,61,62	0
2	SO4	A	292	5/5	0.84	0.14	65,66,67,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LYS	B	292	10/10	0.86	0.15	40,42,44,47	0
2	SO4	B	295	5/5	0.89	0.23	64,65,67,68	0
4	GOL	B	296	6/6	0.89	0.14	46,49,49,50	0
2	SO4	A	293	5/5	0.91	0.23	80,81,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.