



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:24 AM UTC

PDB ID : 2Y52 / pdb_00002y52
Title : Crystal structure of E496A mutant of the box pathway encoded ALDH from Burkholderia xenovorans LB400
Authors : Bains, J.; Leon, R.; Temke, K.G.; Boulanger, M.J.
Deposited on : 2011-01-11
Resolution : 1.65 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

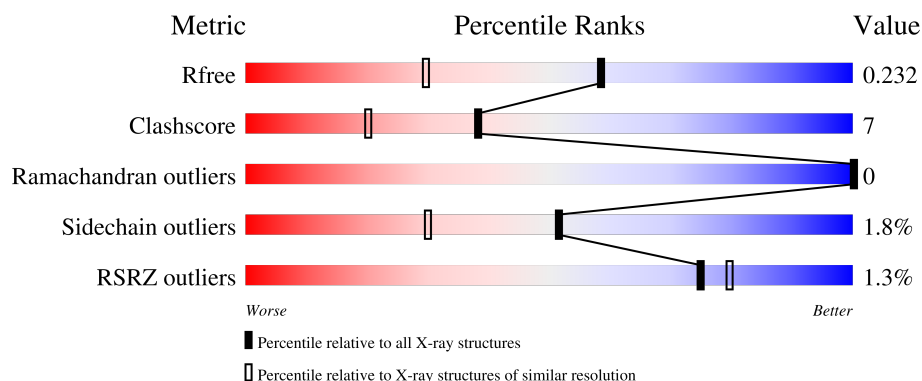
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	534	83% 13% ..
1	B	534	83% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9054 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 ALDEHYDE DEHYDROGENASE (BOX PATHWAY).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3819	2396	690	723	10			
1	B	526	Total	C	N	O	S	0	0	0
			3879	2435	701	733	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q13WK4
A	-1	SER	-	expression tag	UNP Q13WK4
A	0	HIS	-	expression tag	UNP Q13WK4
A	496	ALA	GLU	engineered mutation	UNP Q13WK4
B	-2	GLY	-	expression tag	UNP Q13WK4
B	-1	SER	-	expression tag	UNP Q13WK4
B	0	HIS	-	expression tag	UNP Q13WK4
B	496	ALA	GLU	engineered mutation	UNP Q13WK4

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

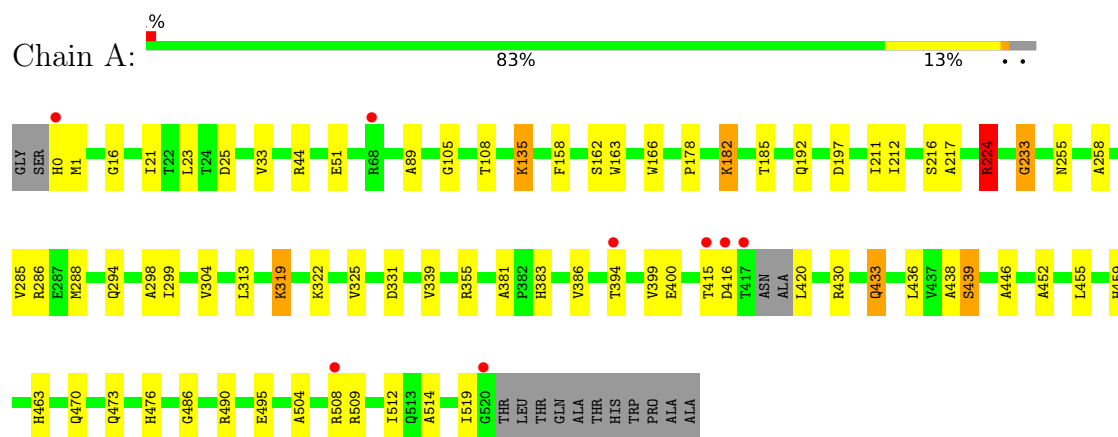
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	674	Total	O	0	0
			674	674		
3	B	658	Total	O	0	0
			658	658		

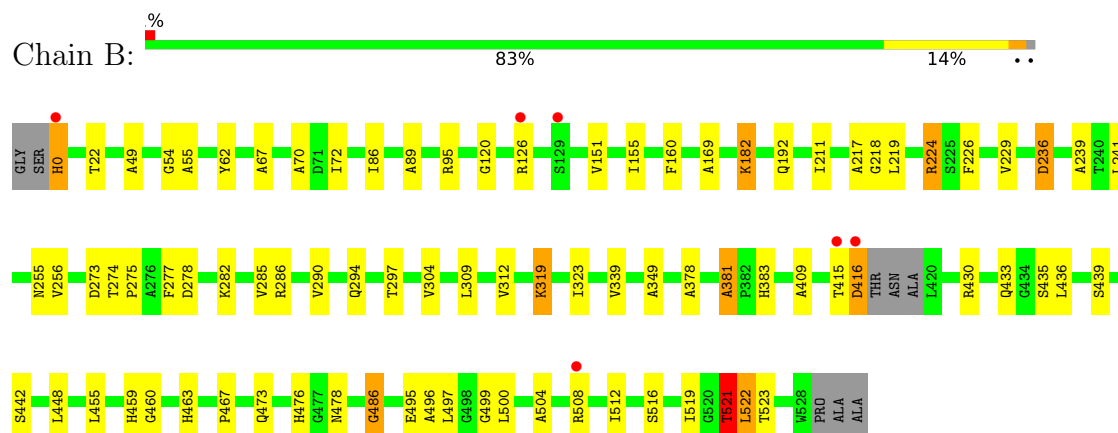
3 Residue-property plots [i](#)

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: ALDEHYDE DEHYDROGENASE (BOX PATHWAY)



• Molecule 1: ALDEHYDE DEHYDROGENASE (BOX PATHWAY)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.05Å 68.13Å 78.08Å 112.23° 90.56° 111.69°	Depositor
Resolution (Å)	38.08 – 1.65 38.08 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (38.08-1.65) 95.9 (38.08-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.180 , 0.231 0.181 , 0.232	Depositor DCC
R_{free} test set	5899 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	9.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9054	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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: 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	1.53	18/3889 (0.5%)	1.23	11/5295 (0.2%)
1	B	1.64	34/3952 (0.9%)	1.29	18/5383 (0.3%)
All	All	1.59	52/7841 (0.7%)	1.26	29/10678 (0.3%)

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 (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	LEU	C-O	-10.79	1.12	1.24
1	B	496	ALA	C-O	-8.43	1.12	1.23
1	B	304	VAL	C-O	-7.46	1.19	1.24
1	B	323	ILE	CA-CB	7.14	1.61	1.53
1	B	486	GLY	N-CA	6.99	1.52	1.45
1	A	21	ILE	C-O	6.58	1.31	1.24
1	B	500	LEU	C-O	-6.50	1.16	1.24
1	A	504	ALA	CA-CB	6.36	1.63	1.53
1	A	486	GLY	N-CA	6.35	1.51	1.45
1	A	394	THR	C-O	6.23	1.29	1.23
1	A	439	SER	N-CA	6.10	1.53	1.45
1	B	522	LEU	CA-CB	6.06	1.62	1.53
1	A	512	ILE	CA-CB	6.06	1.61	1.54
1	A	288	MET	N-CA	6.04	1.54	1.46
1	B	226	PHE	N-CA	6.02	1.53	1.46
1	B	499	GLY	C-O	-5.96	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	VAL	CA-CB	5.83	1.61	1.54
1	B	89	ALA	C-O	5.82	1.31	1.24
1	B	349	ALA	CA-CB	5.80	1.62	1.53
1	B	217	ALA	C-O	5.79	1.30	1.23
1	A	436	LEU	N-CA	5.78	1.53	1.46
1	A	233	GLY	N-CA	5.74	1.51	1.45
1	B	55	ALA	N-CA	5.66	1.53	1.46
1	A	509	ARG	C-O	5.63	1.30	1.23
1	B	70	ALA	CA-CB	5.61	1.62	1.53
1	B	277	PHE	N-CA	5.55	1.52	1.46
1	A	197	ASP	C-O	5.52	1.30	1.24
1	A	400	GLU	N-CA	5.51	1.52	1.46
1	A	212	ILE	C-O	5.50	1.29	1.24
1	B	54	GLY	C-O	5.49	1.30	1.23
1	B	72	ILE	CA-CB	5.46	1.61	1.54
1	B	378	ALA	CA-CB	5.39	1.60	1.53
1	B	62	TYR	C-O	-5.37	1.17	1.24
1	B	22	THR	C-O	5.34	1.30	1.23
1	B	290	VAL	N-CA	5.31	1.52	1.46
1	B	229	VAL	CA-CB	5.31	1.61	1.54
1	B	436	LEU	N-CA	5.26	1.52	1.46
1	B	86	ILE	N-CA	5.26	1.52	1.46
1	A	452	ALA	CA-CB	5.25	1.61	1.53
1	B	155	ILE	CA-CB	5.23	1.60	1.53
1	A	162	SER	CA-C	5.20	1.59	1.53
1	B	182	LYS	CG-CD	-5.14	1.37	1.52
1	B	67	ALA	CA-CB	5.13	1.61	1.53
1	B	312	VAL	C-O	5.12	1.29	1.24
1	A	178	PRO	C-O	5.12	1.29	1.23
1	B	504	ALA	CA-CB	5.09	1.61	1.53
1	A	514	ALA	CA-C	5.08	1.58	1.52
1	B	49	ALA	CA-CB	5.04	1.61	1.53
1	A	325	VAL	CA-CB	5.03	1.61	1.54
1	B	89	ALA	N-CA	5.02	1.52	1.46
1	B	160	PHE	N-CA	5.02	1.52	1.46
1	B	409	ALA	CA-CB	5.01	1.62	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	THR	CA-C-N	7.45	127.32	119.05
1	B	274	THR	C-N-CA	7.45	127.32	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	ALA	CA-C-N	6.98	127.69	119.94
1	B	349	ALA	C-N-CA	6.98	127.69	119.94
1	B	522	LEU	CA-CB-CG	6.84	140.23	116.30
1	A	416	ASP	N-CA-C	6.24	119.64	109.59
1	A	394	THR	CB-CA-C	-6.19	100.93	112.00
1	B	521	THR	N-CA-CB	6.14	119.24	110.16
1	A	508	ARG	NE-CZ-NH2	-6.04	113.77	119.20
1	B	236	ASP	CB-CA-C	-5.99	101.39	110.92
1	B	239	ALA	N-CA-C	5.95	117.84	111.36
1	B	169	ALA	CA-C-N	-5.92	113.25	119.83
1	B	169	ALA	C-N-CA	-5.92	113.25	119.83
1	A	185	THR	N-CA-C	5.65	117.44	111.28
1	B	218	GLY	N-CA-C	5.59	122.78	115.40
1	A	304	VAL	CA-C-N	-5.53	114.08	119.78
1	A	304	VAL	C-N-CA	-5.53	114.08	119.78
1	A	166	TRP	N-CA-C	5.50	118.20	111.82
1	B	455	LEU	N-CA-C	-5.48	106.60	113.72
1	A	399	VAL	N-CA-C	5.47	115.67	107.51
1	A	455	LEU	N-CA-C	-5.39	106.72	113.72
1	A	16	GLY	N-CA-C	-5.32	105.74	112.54
1	B	151	VAL	CB-CA-C	-5.29	103.63	111.19
1	B	415	THR	CB-CA-C	5.22	119.32	111.18
1	A	224	ARG	CB-CG-CD	5.14	123.13	111.30
1	B	381	ALA	CA-C-N	-5.08	114.52	119.76
1	B	381	ALA	C-N-CA	-5.08	114.52	119.76
1	B	433	GLN	CB-CA-C	-5.06	103.51	111.51
1	B	309	LEU	N-CA-C	5.03	116.45	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	519	ILE	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	3819	0	3828	61	0
1	B	3879	0	3883	46	1
2	A	12	0	15	0	0
2	B	12	0	16	0	0
3	A	674	0	0	28	0
3	B	658	0	0	13	1
All	All	9054	0	7742	106	1

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 7.

All (106) 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:51:GLU:HG2	3:A:2064:HOH:O	1.59	1.03
1:A:105:GLY:HA2	3:A:2260:HOH:O	1.64	0.96
1:B:286:ARG:NH2	1:B:478:ASN:HD21	1.68	0.91
1:A:0:HIS:HA	1:A:1:MET:HG3	1.54	0.89
1:A:0:HIS:HA	1:A:1:MET:CG	2.03	0.88
1:A:286:ARG:NH1	3:A:2462:HOH:O	1.99	0.88
1:A:255:ASN:HD21	1:A:495:GLU:H	1.21	0.87
1:A:331:ASP:OD1	3:A:2506:HOH:O	1.94	0.85
1:B:286:ARG:HH22	1:B:478:ASN:HD21	1.27	0.83
1:B:430:ARG:NH2	3:B:2576:HOH:O	2.06	0.81
1:A:135:LYS:HA	1:A:135:LYS:HE2	1.63	0.79
1:B:286:ARG:HH22	1:B:478:ASN:ND2	1.83	0.77
1:B:519:ILE:O	1:B:523:THR:HG23	1.84	0.77
1:B:255:ASN:HD21	1:B:495:GLU:H	1.33	0.75
1:A:476:HIS:ND1	3:A:2635:HOH:O	2.20	0.75
1:A:298:ALA:HA	3:A:2635:HOH:O	1.87	0.74
1:B:519:ILE:HA	1:B:522:LEU:HD12	1.70	0.73
1:B:278:ASP:OD2	1:B:282:LYS:HE3	1.88	0.73
1:A:420:LEU:HD21	3:A:2354:HOH:O	1.88	0.72
1:B:416:ASP:HB3	3:B:2567:HOH:O	1.89	0.71
1:A:476:HIS:CE1	3:A:2635:HOH:O	2.45	0.69
1:B:286:ARG:NH2	1:B:478:ASN:ND2	2.40	0.68
1:A:430:ARG:HG3	3:A:2622:HOH:O	1.93	0.68
1:A:163:TRP:HD1	3:A:2260:HOH:O	1.76	0.67
1:B:319:LYS:HB2	1:B:319:LYS:NZ	2.09	0.67
1:A:319:LYS:HB2	1:A:319:LYS:NZ	2.11	0.66
1:A:163:TRP:CD1	3:A:2260:HOH:O	2.48	0.65
1:A:381:ALA:O	1:A:383:HIS:HD2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LYS:HG3	3:A:2491:HOH:O	1.96	0.64
1:B:0:HIS:HB3	3:B:2006:HOH:O	1.97	0.63
1:B:224:ARG:CG	1:B:224:ARG:HH11	2.11	0.63
1:A:135:LYS:HA	1:A:135:LYS:CE	2.30	0.61
1:A:490:ARG:NE	3:A:2644:HOH:O	2.35	0.60
1:B:523:THR:HG21	3:B:2298:HOH:O	2.04	0.58
1:B:297:THR:O	1:B:476:HIS:HE1	1.86	0.58
1:A:439:SER:OG	1:A:476:HIS:HD2	1.85	0.58
1:B:381:ALA:O	1:B:383:HIS:HD2	1.86	0.58
1:B:294:GLN:HE22	1:B:339:VAL:H	1.50	0.58
1:B:521:THR:HG22	3:B:2644:HOH:O	2.03	0.57
1:A:299:ILE:N	3:A:2635:HOH:O	2.36	0.57
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.70	0.57
1:A:294:GLN:HE22	1:A:339:VAL:H	1.52	0.56
1:B:120:GLY:HA3	3:B:2651:HOH:O	2.06	0.55
1:B:519:ILE:HD13	1:B:522:LEU:CD1	2.36	0.55
1:A:319:LYS:HB2	1:A:319:LYS:HZ3	1.70	0.55
1:A:255:ASN:HD21	1:A:495:GLU:N	2.00	0.55
1:A:0:HIS:ND1	1:A:0:HIS:O	2.40	0.54
1:A:224:ARG:HH11	1:A:224:ARG:CG	2.20	0.54
1:B:442:SER:HB3	1:B:448:LEU:HD21	1.88	0.54
1:A:433:GLN:HG3	1:A:490:ARG:CZ	2.38	0.54
1:B:383:HIS:HE1	3:B:2505:HOH:O	1.90	0.53
1:A:470:GLN:NE2	3:A:2628:HOH:O	2.42	0.53
1:A:158:PHE:CD1	1:A:339:VAL:HG21	2.44	0.53
1:A:430:ARG:HD2	3:A:2604:HOH:O	2.09	0.53
1:B:519:ILE:HD13	1:B:522:LEU:HD12	1.91	0.51
1:A:0:HIS:O	1:A:0:HIS:CG	2.63	0.51
1:A:285:VAL:HG11	1:A:319:LYS:HG2	1.92	0.51
1:B:297:THR:O	1:B:476:HIS:CE1	2.65	0.50
1:B:285:VAL:HG11	1:B:319:LYS:HG2	1.93	0.50
1:B:439:SER:OG	1:B:476:HIS:HD2	1.94	0.50
1:A:439:SER:CB	1:A:476:HIS:HD2	2.25	0.50
1:A:51:GLU:HG2	3:A:2154:HOH:O	2.11	0.49
1:B:286:ARG:CZ	3:B:2435:HOH:O	2.59	0.49
1:B:439:SER:CB	1:B:476:HIS:HD2	2.25	0.49
1:A:192:GLN:HA	1:A:211:ILE:HD13	1.93	0.49
1:B:319:LYS:NZ	1:B:319:LYS:CB	2.75	0.49
1:A:420:LEU:CD2	3:A:2354:HOH:O	2.53	0.48
1:B:273:ASP:CG	3:B:2426:HOH:O	2.55	0.48
1:A:298:ALA:CA	3:A:2635:HOH:O	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:CG	3:A:2154:HOH:O	2.62	0.47
1:A:313:LEU:HD21	1:A:386:VAL:HG22	1.95	0.47
1:B:126:ARG:NH2	3:B:2266:HOH:O	2.47	0.47
1:B:182:LYS:HG3	1:B:219:LEU:HD11	1.96	0.47
1:A:233:GLY:O	1:A:258:ALA:HA	2.15	0.47
1:A:355:ARG:NH1	3:A:2534:HOH:O	2.45	0.46
1:B:460:GLY:HA3	1:B:486:GLY:O	2.14	0.46
1:A:224:ARG:HH11	1:A:224:ARG:HG3	1.80	0.46
1:B:319:LYS:HG3	3:B:2459:HOH:O	2.15	0.45
1:A:25:ASP:HA	1:A:89:ALA:O	2.17	0.45
1:A:298:ALA:C	3:A:2635:HOH:O	2.58	0.45
1:A:322:LYS:HD2	3:A:2490:HOH:O	2.16	0.45
1:A:430:ARG:NH1	3:A:2604:HOH:O	2.48	0.45
1:B:236:ASP:CG	3:B:2391:HOH:O	2.59	0.45
1:A:439:SER:OG	1:A:476:HIS:CD2	2.68	0.45
1:A:433:GLN:HG3	1:A:490:ARG:NH2	2.32	0.44
1:A:108:THR:HB	3:A:2260:HOH:O	2.17	0.44
1:A:446:ALA:HA	1:B:521:THR:HG21	2.00	0.44
1:B:463:HIS:HE1	1:B:473:GLN:OE1	2.01	0.43
1:A:0:HIS:CA	1:A:1:MET:HG3	2.36	0.43
1:B:95:ARG:HD2	3:B:2217:HOH:O	2.18	0.43
1:B:512:ILE:HG21	1:B:522:LEU:HD21	2.01	0.43
1:B:275:PRO:HB2	1:B:467:PRO:HG3	2.01	0.43
1:A:463:HIS:HE1	1:A:473:GLN:OE1	2.02	0.43
1:B:192:GLN:HA	1:B:211:ILE:HD13	2.01	0.42
1:B:319:LYS:HB2	1:B:319:LYS:HZ3	1.80	0.41
1:B:439:SER:HB3	1:B:476:HIS:HD2	1.84	0.41
1:B:182:LYS:HG3	1:B:219:LEU:CD1	2.51	0.41
1:A:383:HIS:HE1	3:A:2545:HOH:O	2.02	0.41
1:B:435:SER:HB2	1:B:459:HIS:CD2	2.55	0.41
1:A:438:ALA:HB2	1:A:459:HIS:CD2	2.56	0.41
1:A:319:LYS:NZ	1:A:319:LYS:CB	2.78	0.40
1:A:23:LEU:HD22	1:A:33:VAL:HG23	2.03	0.40
1:A:224:ARG:CG	1:A:224:ARG:NH1	2.84	0.40
1:A:182:LYS:HD2	3:A:2360:HOH:O	2.22	0.40
1:A:216:SER:O	1:A:217:ALA:C	2.65	0.40
1:A:331:ASP:HB2	3:A:2504:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:SER:CB	3:B:2391:HOH:O[1_655]	1.83	0.37

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	515/534 (96%)	507 (98%)	8 (2%)	0	100	100
1	B	522/534 (98%)	511 (98%)	11 (2%)	0	100	100
All	All	1037/1068 (97%)	1018 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	388/398 (98%)	381 (98%)	7 (2%)	51	30
1	B	394/398 (99%)	387 (98%)	7 (2%)	51	30
All	All	782/796 (98%)	768 (98%)	14 (2%)	51	30

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

Mol	Chain	Res	Type
1	A	44	ARG
1	A	135	LYS
1	A	182	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	224	ARG
1	A	319	LYS
1	A	415	THR
1	A	433	GLN
1	B	0	HIS
1	B	224	ARG
1	B	241	LEU
1	B	319	LYS
1	B	416	ASP
1	B	508	ARG
1	B	521	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	77	GLN
1	A	255	ASN
1	A	294	GLN
1	A	343	GLN
1	A	346	ASN
1	A	383	HIS
1	A	463	HIS
1	A	470	GLN
1	A	476	HIS
1	B	8	HIS
1	B	90	ASN
1	B	123	HIS
1	B	142	GLN
1	B	255	ASN
1	B	294	GLN
1	B	343	GLN
1	B	346	ASN
1	B	383	HIS
1	B	433	GLN
1	B	463	HIS
1	B	476	HIS
1	B	478	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
2	GOL	A	1521	-	5,5,5	0.89	0	5,5,5	1.69	2 (40%)
2	GOL	B	1529	-	5,5,5	0.49	0	5,5,5	0.36	0
2	GOL	A	1522	-	5,5,5	0.40	0	5,5,5	0.65	0
2	GOL	B	1530	-	5,5,5	0.67	0	5,5,5	0.97	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	GOL	A	1521	-	-	3/4/4/4	-
2	GOL	B	1529	-	-	0/4/4/4	-
2	GOL	A	1522	-	-	0/4/4/4	-
2	GOL	B	1530	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1521	GOL	O2-C2-C1	2.70	120.34	109.18
2	A	1521	GOL	C3-C2-C1	2.12	119.57	111.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1521	GOL	O1-C1-C2-C3
2	A	1521	GOL	O1-C1-C2-O2
2	A	1521	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	519/534 (97%)	-0.39	8 (1%) 72 77	2, 10, 21, 47	2 (0%)
1	B	526/534 (98%)	-0.47	6 (1%) 78 83	1, 9, 17, 45	3 (0%)
All	All	1045/1068 (97%)	-0.43	14 (1%) 75 80	1, 9, 20, 47	5 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	THR	5.3
1	B	416	ASP	4.0
1	A	520	GLY	3.9
1	B	129	SER	3.8
1	B	415	THR	3.7
1	A	0	HIS	3.3
1	A	68	ARG	3.1
1	B	0	HIS	2.9
1	B	126	ARG	2.9
1	A	508	ARG	2.7
1	B	508	ARG	2.5
1	A	416	ASP	2.4
1	A	394	THR	2.3
1	A	415	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($\text{\AA}^2$)	Q<0.9
2	GOL	B	1530	6/6	0.95	0.08	9,15,17,19	0
2	GOL	A	1522	6/6	0.96	0.07	12,15,17,18	0
2	GOL	A	1521	6/6	0.97	0.05	10,13,14,16	0
2	GOL	B	1529	6/6	0.98	0.05	10,13,13,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.