



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:43 PM UTC

PDB ID : 2Y51 / pdb_00002y51
Title : Crystal structure of E167A 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 : 1.60 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

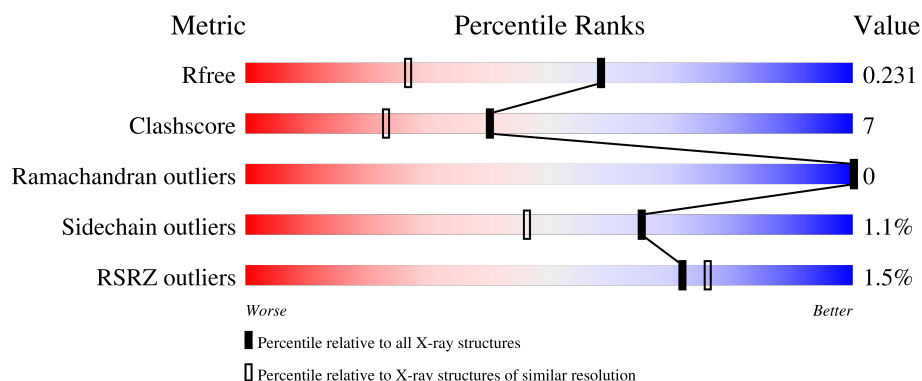
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	534	% 87% 11% ..
1	B	534	2% 83% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8943 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	529	Total	C	N	O	S	0	0	0
			3899	2446	705	738	10			
1	B	528	Total	C	N	O	S	0	0	0
			3891	2442	703	736	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	167	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	167	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		

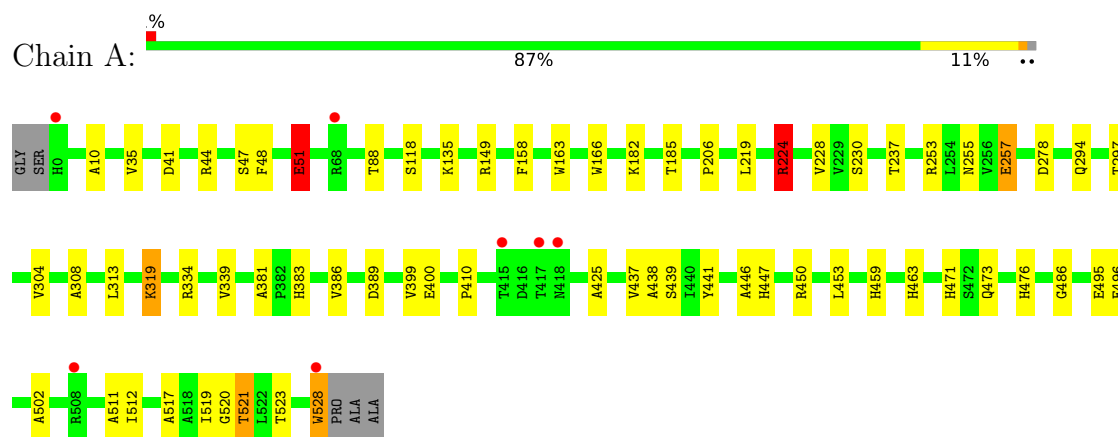
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	537	Total	O	0	0
			537	537		
3	B	592	Total	O	0	0
			592	592		

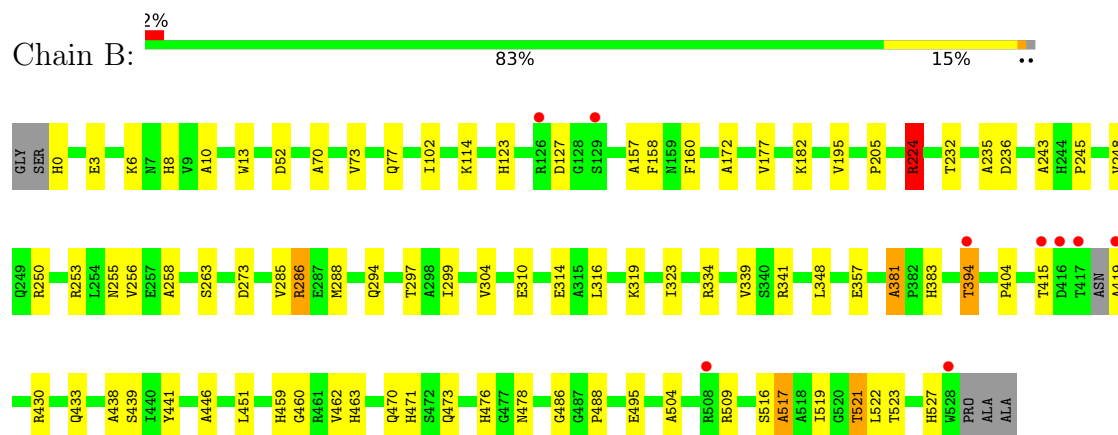
3 Residue-property plots

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: 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	57.59Å 67.63Å 77.27Å 112.48° 90.14° 111.51°	Depositor
Resolution (Å)	37.72 – 1.60 37.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.4 (37.72-1.60) 93.4 (37.72-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.179 , 0.230 0.181 , 0.231	Depositor DCC
R_{free} test set	6137 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	8.2	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8943	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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

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	1.48	20/3973 (0.5%)	1.22	8/5414 (0.1%)
1	B	1.57	27/3964 (0.7%)	1.27	11/5400 (0.2%)
All	All	1.52	47/7937 (0.6%)	1.25	19/10814 (0.2%)

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	B	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	VAL	C-O	-9.56	1.17	1.24
1	A	486	GLY	N-CA	9.16	1.53	1.45
1	B	256	VAL	CA-CB	6.92	1.64	1.54
1	A	51	GLU	CA-C	-6.84	1.44	1.53
1	A	425	ALA	CA-CB	-6.79	1.42	1.53
1	A	228	VAL	C-O	6.74	1.30	1.24
1	B	172	ALA	CA-CB	6.67	1.63	1.53
1	B	157	ALA	N-CA	6.61	1.54	1.45
1	B	394	THR	CA-CB	6.33	1.63	1.53
1	A	511	ALA	N-CA	6.30	1.53	1.46
1	A	230	SER	N-CA	6.21	1.53	1.46
1	A	437	VAL	CA-CB	6.21	1.61	1.55
1	A	253	ARG	CB-CG	-6.18	1.33	1.52
1	B	160	PHE	N-CA	5.96	1.53	1.46
1	B	323	ILE	C-O	5.95	1.30	1.23
1	B	102	ILE	N-CA	5.82	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	517	ALA	CA-CB	5.71	1.62	1.53
1	B	286	ARG	CA-C	5.69	1.60	1.52
1	B	253	ARG	CB-CG	-5.64	1.35	1.52
1	B	504	ALA	CA-CB	5.63	1.62	1.53
1	A	35	VAL	CA-CB	5.62	1.64	1.54
1	B	235	ALA	N-CA	5.53	1.53	1.46
1	B	10	ALA	CA-CB	-5.42	1.44	1.53
1	B	316	LEU	N-CA	5.31	1.52	1.46
1	B	263	SER	N-CA	-5.30	1.39	1.45
1	B	182	LYS	CG-CD	-5.27	1.36	1.52
1	A	237	THR	CA-CB	5.27	1.61	1.53
1	B	415	THR	CA-CB	5.25	1.60	1.53
1	B	299	ILE	CA-C	5.25	1.58	1.52
1	B	195	VAL	CA-CB	5.24	1.60	1.54
1	B	243	ALA	CA-CB	5.23	1.62	1.53
1	A	51	GLU	CB-CG	-5.21	1.36	1.52
1	B	177	VAL	CA-CB	5.20	1.61	1.54
1	B	232	THR	N-CA	5.20	1.52	1.46
1	A	278	ASP	C-O	5.19	1.30	1.24
1	A	502	ALA	N-CA	5.17	1.52	1.46
1	B	258	ALA	C-O	-5.13	1.18	1.24
1	A	206	PRO	C-O	5.10	1.29	1.23
1	A	400	GLU	N-CA	5.10	1.52	1.46
1	A	118	SER	CA-C	5.07	1.59	1.52
1	B	70	ALA	CA-CB	5.06	1.61	1.53
1	A	163	TRP	C-O	-5.05	1.18	1.24
1	B	488	PRO	N-CA	5.05	1.52	1.47
1	A	149	ARG	C-O	5.05	1.29	1.23
1	A	308	ALA	CA-CB	-5.04	1.45	1.53
1	B	451	LEU	C-O	5.01	1.29	1.24
1	A	257	GLU	CA-C	-5.00	1.46	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	ALA	CA-C-N	-8.03	111.49	119.76
1	B	381	ALA	C-N-CA	-8.03	111.49	119.76
1	B	102	ILE	N-CA-C	7.89	117.95	110.30
1	A	486	GLY	N-CA-C	-6.60	101.11	110.88
1	B	341	ARG	CG-CD-NE	-6.45	97.80	112.00
1	A	389	ASP	CA-C-N	-5.93	113.58	119.56
1	A	389	ASP	C-N-CA	-5.93	113.58	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	PRO	CB-CA-C	-5.43	106.29	111.39
1	B	3	GLU	N-CA-C	5.36	118.12	110.24
1	B	250	ARG	N-CA-C	5.35	119.86	113.23
1	A	224	ARG	CB-CG-CD	5.33	123.57	111.30
1	B	224	ARG	CG-CD-NE	5.33	123.73	112.00
1	A	185	THR	N-CA-C	5.23	116.66	111.07
1	B	516	SER	N-CA-C	5.14	117.55	111.33
1	B	273	ASP	N-CA-C	5.13	119.29	113.19
1	A	88	THR	O-C-N	5.09	127.32	122.07
1	B	52	ASP	N-CA-C	5.04	116.58	111.14
1	A	399	VAL	N-CA-C	5.02	114.99	107.51
1	A	166	TRP	N-CA-C	5.01	117.63	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	527	HIS	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	3899	0	3902	48	0
1	B	3891	0	3895	59	0
2	A	12	0	16	0	0
2	B	12	0	16	0	0
3	A	537	0	0	15	1
3	B	592	0	0	20	3
All	All	8943	0	7829	103	3

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 (103) 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:528:TRP:CZ3	3:A:2199:HOH:O	2.02	1.09
1:B:127:ASP:OD2	1:B:509:ARG:NH1	1.89	1.05
1:B:286:ARG:NH2	1:B:478:ASN:HD21	1.59	1.01
1:B:6:LYS:HE2	3:B:2022:HOH:O	1.65	0.94
1:A:528:TRP:CH2	3:A:2199:HOH:O	2.17	0.94
1:B:286:ARG:HH22	1:B:478:ASN:HD21	1.11	0.90
1:B:255:ASN:HD21	1:B:495:GLU:H	1.16	0.89
1:B:286:ARG:HH22	1:B:478:ASN:ND2	1.71	0.87
1:A:519:ILE:O	1:A:523:THR:HG23	1.79	0.81
1:A:255:ASN:HD21	1:A:495:GLU:H	1.28	0.80
1:B:236:ASP:C	3:B:2345:HOH:O	2.24	0.80
1:B:357:GLU:O	1:B:357:GLU:HG2	1.81	0.80
1:B:519:ILE:HA	1:B:522:LEU:HD12	1.64	0.80
1:B:519:ILE:O	1:B:523:THR:HG23	1.82	0.80
1:A:450:ARG:NH2	3:A:2482:HOH:O	2.16	0.79
1:A:224:ARG:HH11	1:A:224:ARG:CG	1.96	0.77
1:B:357:GLU:OE1	1:B:394:THR:OG1	2.02	0.77
1:B:314:GLU:HG2	3:B:2402:HOH:O	1.88	0.73
1:A:313:LEU:HD21	1:A:386:VAL:HG22	1.71	0.72
1:B:357:GLU:O	1:B:357:GLU:CG	2.41	0.69
1:B:6:LYS:CE	3:B:2022:HOH:O	2.31	0.68
1:A:450:ARG:HD3	3:A:2483:HOH:O	1.93	0.67
1:A:41:ASP:OD2	3:A:2075:HOH:O	2.14	0.66
1:B:439:SER:OG	1:B:476:HIS:HD2	1.79	0.66
3:A:2226:HOH:O	1:B:430:ARG:HD3	1.95	0.66
1:A:294:GLN:HE22	1:A:339:VAL:H	1.44	0.65
1:A:224:ARG:HH11	1:A:224:ARG:HG3	1.61	0.64
1:B:286:ARG:NH2	1:B:478:ASN:ND2	2.35	0.64
1:B:73:VAL:O	1:B:77:GLN:HG3	1.98	0.64
1:A:450:ARG:CD	3:A:2483:HOH:O	2.44	0.63
1:A:224:ARG:HH11	1:A:224:ARG:HG2	1.61	0.63
1:B:383:HIS:HE1	3:B:2457:HOH:O	1.81	0.62
1:A:334:ARG:HD3	3:A:2381:HOH:O	1.98	0.62
1:A:381:ALA:O	1:A:383:HIS:HD2	1.83	0.61
1:A:224:ARG:CG	1:A:224:ARG:NH1	2.62	0.57
1:A:224:ARG:HG2	1:A:224:ARG:NH1	2.18	0.57
1:B:523:THR:HG21	3:B:2260:HOH:O	2.05	0.56
1:A:520:GLY:O	1:A:523:THR:OG1	2.24	0.56
1:B:114:LYS:HE2	3:B:2038:HOH:O	2.04	0.55
1:A:44:ARG:HD2	3:A:2082:HOH:O	2.05	0.55
1:B:419:ALA:HB1	3:B:2508:HOH:O	2.07	0.55
1:B:463:HIS:HE1	1:B:473:GLN:OE1	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ALA:O	1:B:521:THR:HG23	2.06	0.55
1:B:224:ARG:CG	1:B:224:ARG:HH11	2.20	0.54
1:A:257:GLU:OE2	1:A:496:GLU:OE2	2.26	0.54
1:A:47:SER:O	1:A:51:GLU:HG2	2.07	0.54
1:A:453:LEU:HG	1:B:522:LEU:HD23	1.90	0.54
1:B:285:VAL:HG21	1:B:319:LYS:HB3	1.90	0.54
1:B:381:ALA:O	1:B:383:HIS:HD2	1.91	0.53
1:A:439:SER:OG	1:A:476:HIS:HD2	1.91	0.53
1:A:313:LEU:HD21	1:A:386:VAL:CG2	2.38	0.52
1:A:521:THR:HG22	3:A:2530:HOH:O	2.08	0.52
1:B:294:GLN:HE22	1:B:339:VAL:H	1.57	0.52
1:B:334:ARG:NH1	3:B:2426:HOH:O	2.43	0.51
1:B:255:ASN:HD21	1:B:495:GLU:N	1.95	0.51
1:A:517:ALA:O	1:A:521:THR:HG23	2.10	0.51
1:B:348:LEU:HD22	3:B:2229:HOH:O	2.09	0.50
1:B:470:GLN:HG3	1:B:471:HIS:N	2.27	0.50
1:B:470:GLN:CD	3:B:2545:HOH:O	2.54	0.49
1:B:0:HIS:CD2	1:B:0:HIS:N	2.81	0.49
1:B:297:THR:O	1:B:476:HIS:CE1	2.66	0.49
1:A:523:THR:CG2	3:A:2223:HOH:O	2.62	0.48
1:B:123:HIS:HE1	3:B:2225:HOH:O	1.97	0.48
1:B:460:GLY:HA3	1:B:486:GLY:O	2.13	0.48
1:A:439:SER:CB	1:A:476:HIS:HD2	2.26	0.48
1:B:245:PRO:HA	1:B:248:VAL:HG22	1.96	0.48
1:B:297:THR:O	1:B:476:HIS:HE1	1.96	0.48
1:A:10:ALA:HA	1:A:48:PHE:CD2	2.48	0.48
1:A:319:LYS:HB2	1:A:319:LYS:HE2	1.34	0.48
1:B:236:ASP:CB	3:B:2345:HOH:O	2.62	0.47
1:A:51:GLU:HG2	1:A:51:GLU:H	1.52	0.47
1:A:446:ALA:HA	1:B:521:THR:HG21	1.97	0.46
1:A:523:THR:HG21	3:A:2223:HOH:O	2.15	0.46
1:B:441:TYR:N	1:B:441:TYR:CD1	2.84	0.46
1:A:438:ALA:HB2	1:A:459:HIS:CD2	2.51	0.46
1:B:158:PHE:CD1	1:B:339:VAL:HG21	2.50	0.46
1:B:286:ARG:CZ	3:B:2379:HOH:O	2.64	0.46
1:A:383:HIS:HE1	3:A:2415:HOH:O	1.99	0.46
1:B:286:ARG:NE	3:B:2380:HOH:O	2.49	0.46
1:B:439:SER:HA	1:B:463:HIS:O	2.17	0.45
1:B:439:SER:CB	1:B:476:HIS:HD2	2.30	0.45
1:A:158:PHE:CD1	1:A:339:VAL:HG21	2.52	0.45
1:A:447:HIS:ND1	1:A:450:ARG:NH1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:HIS:HB2	1:B:13:TRP:CZ3	2.53	0.44
1:A:304:VAL:O	1:A:410:PRO:HA	2.18	0.44
1:A:439:SER:HA	1:A:463:HIS:O	2.17	0.44
1:B:438:ALA:HB2	1:B:459:HIS:CD2	2.52	0.44
1:B:236:ASP:HB2	3:B:2345:HOH:O	2.17	0.44
1:B:439:SER:OG	1:B:476:HIS:CD2	2.65	0.44
1:A:441:TYR:CD1	1:A:441:TYR:N	2.86	0.44
1:B:286:ARG:NH1	3:B:2379:HOH:O	2.51	0.43
1:A:463:HIS:HE1	1:A:473:GLN:OE1	2.02	0.43
1:A:471:HIS:HB3	3:A:2495:HOH:O	2.18	0.42
1:A:182:LYS:HG3	1:A:219:LEU:HD11	2.00	0.42
1:A:297:THR:O	1:A:476:HIS:CE1	2.73	0.42
1:A:512:ILE:HD12	1:B:462:VAL:HB	2.03	0.41
1:B:288:MET:O	1:B:404:PRO:HA	2.21	0.41
1:B:433:GLN:HG3	3:B:2517:HOH:O	2.20	0.41
1:A:319:LYS:HD3	3:A:2183:HOH:O	2.21	0.41
1:A:313:LEU:CD2	1:A:386:VAL:CG2	2.98	0.40
1:B:433:GLN:CG	3:B:2517:HOH:O	2.70	0.40
1:B:286:ARG:HD3	3:B:2201:HOH:O	2.22	0.40
1:A:521:THR:HG21	1:B:446:ALA:HA	2.03	0.40

All (3) 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)
3:B:2034:HOH:O	3:B:2483:HOH:O[1_545]	2.08	0.12
3:A:2369:HOH:O	3:B:2405:HOH:O[1_656]	2.12	0.08
3:B:2116:HOH:O	3:B:2391:HOH:O[1_545]	2.13	0.07

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	527/534 (99%)	520 (99%)	7 (1%)	0	100	100
1	B	524/534 (98%)	512 (98%)	12 (2%)	0	100	100
All	All	1051/1068 (98%)	1032 (98%)	19 (2%)	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	396/398 (100%)	390 (98%)	6 (2%)	57	35
1	B	395/398 (99%)	392 (99%)	3 (1%)	73	59
All	All	791/796 (99%)	782 (99%)	9 (1%)	65	46

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	135	LYS
1	A	224	ARG
1	A	319	LYS
1	A	521	THR
1	A	528	TRP
1	B	224	ARG
1	B	310	GLU
1	B	521	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	90	ASN
1	A	123	HIS
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	255	ASN
1	A	294	GLN
1	A	343	GLN
1	A	346	ASN
1	A	383	HIS
1	A	392	ASN
1	A	463	HIS
1	A	476	HIS
1	A	527	HIS
1	B	0	HIS
1	B	8	HIS
1	B	77	GLN
1	B	123	HIS
1	B	142	GLN
1	B	255	ASN
1	B	294	GLN
1	B	346	ASN
1	B	375	ASN
1	B	383	HIS
1	B	463	HIS
1	B	476	HIS
1	B	478	ASN

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](#)

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	B	1529	-	5,5,5	0.63	0	5,5,5	0.58	0
2	GOL	A	1530	-	5,5,5	0.29	0	5,5,5	0.96	0
2	GOL	A	1529	-	5,5,5	0.63	0	5,5,5	0.51	0
2	GOL	B	1530	-	5,5,5	0.58	0	5,5,5	0.77	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	B	1529	-	-	0/4/4/4	-
2	GOL	A	1530	-	-	0/4/4/4	-
2	GOL	A	1529	-	-	1/4/4/4	-
2	GOL	B	1530	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1529	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 ⓘ

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	529/534 (99%)	-0.51	7 (1%) 75 79	2, 10, 23, 44	2 (0%)
1	B	528/534 (98%)	-0.56	9 (1%) 69 72	2, 9, 19, 49	3 (0%)
All	All	1057/1068 (98%)	-0.53	16 (1%) 72 76	2, 10, 21, 49	5 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	THR	6.8
1	A	528	TRP	4.6
1	B	415	THR	4.4
1	B	129	SER	4.0
1	A	418	ASN	3.4
1	B	416	ASP	3.2
1	B	394	THR	3.1
1	A	68	ARG	3.1
1	A	508	ARG	3.0
1	A	417	THR	3.0
1	B	508	ARG	2.8
1	B	126	ARG	2.7
1	B	528	TRP	2.4
1	B	419	ALA	2.3
1	A	415	THR	2.2
1	A	0	HIS	2.1

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	0.93	0.09	13,20,22,22	0
2	GOL	A	1530	6/6	0.97	0.07	10,19,21,24	0
2	GOL	B	1529	6/6	0.98	0.04	10,12,13,14	0
2	GOL	A	1529	6/6	0.98	0.04	10,12,13,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.