



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:42 PM UTC

PDB ID : 5CEF / pdb_00005cef
Title : Crystal structure of aspartate semialdehyde dehydrogenase from *Cryptococcus neoformans*
Authors : Dahal, G.P.; Viola, R.E.
Deposited on : 2015-07-06
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

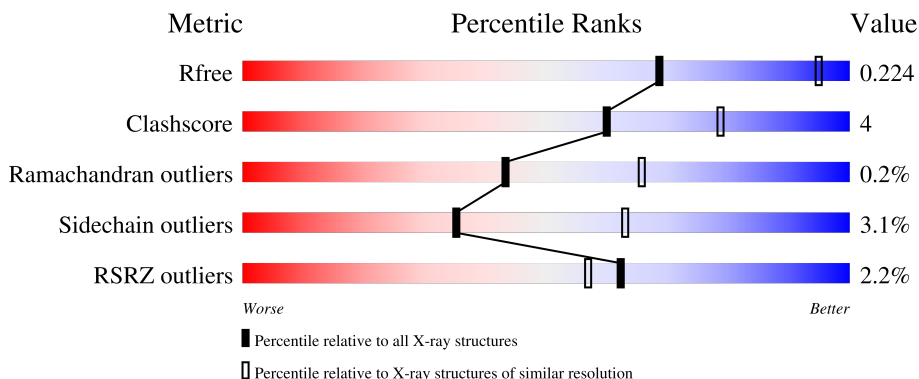
1 Overall quality at a glance

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)
Ramachandran outliers	187476	4277 (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	375	 87% 8% . .
1	B	375	 86% 10% .
1	C	375	 86% 9% . .
1	D	375	 85% 10% . .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 11419 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 Aspartate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2699	1707	479	501	12	0	0	0
1	B	359	2699	1707	479	501	12	0	0	0
1	C	359	2699	1707	479	501	12	0	0	0
1	D	359	2699	1707	479	501	12	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q5KPK7
A	0	GLY	-	expression tag	UNP Q5KPK7
A	366	LEU	-	expression tag	UNP Q5KPK7
A	367	GLU	-	expression tag	UNP Q5KPK7
A	368	HIS	-	expression tag	UNP Q5KPK7
A	369	HIS	-	expression tag	UNP Q5KPK7
A	370	HIS	-	expression tag	UNP Q5KPK7
A	371	HIS	-	expression tag	UNP Q5KPK7
A	372	HIS	-	expression tag	UNP Q5KPK7
A	373	HIS	-	expression tag	UNP Q5KPK7
B	-1	MET	-	initiating methionine	UNP Q5KPK7
B	0	GLY	-	expression tag	UNP Q5KPK7
B	366	LEU	-	expression tag	UNP Q5KPK7
B	367	GLU	-	expression tag	UNP Q5KPK7
B	368	HIS	-	expression tag	UNP Q5KPK7
B	369	HIS	-	expression tag	UNP Q5KPK7
B	370	HIS	-	expression tag	UNP Q5KPK7
B	371	HIS	-	expression tag	UNP Q5KPK7
B	372	HIS	-	expression tag	UNP Q5KPK7
B	373	HIS	-	expression tag	UNP Q5KPK7
C	-1	MET	-	initiating methionine	UNP Q5KPK7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q5KPK7
C	366	LEU	-	expression tag	UNP Q5KPK7
C	367	GLU	-	expression tag	UNP Q5KPK7
C	368	HIS	-	expression tag	UNP Q5KPK7
C	369	HIS	-	expression tag	UNP Q5KPK7
C	370	HIS	-	expression tag	UNP Q5KPK7
C	371	HIS	-	expression tag	UNP Q5KPK7
C	372	HIS	-	expression tag	UNP Q5KPK7
C	373	HIS	-	expression tag	UNP Q5KPK7
D	-1	MET	-	initiating methionine	UNP Q5KPK7
D	0	GLY	-	expression tag	UNP Q5KPK7
D	366	LEU	-	expression tag	UNP Q5KPK7
D	367	GLU	-	expression tag	UNP Q5KPK7
D	368	HIS	-	expression tag	UNP Q5KPK7
D	369	HIS	-	expression tag	UNP Q5KPK7
D	370	HIS	-	expression tag	UNP Q5KPK7
D	371	HIS	-	expression tag	UNP Q5KPK7
D	372	HIS	-	expression tag	UNP Q5KPK7
D	373	HIS	-	expression tag	UNP Q5KPK7

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
2	A	1	4	2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total 198	O 198	0	0
3	B	122	Total 122	O 122	0	0
3	C	168	Total 168	O 168	0	0
3	D	131	Total 131	O 131	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.59Å 130.96Å 91.94Å 90.00° 92.87° 90.00°	Depositor
Resolution (Å)	66.05 – 2.60 66.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.05-2.60) 100.0 (66.05-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.62Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.181 , 0.220 0.187 , 0.224	Depositor DCC
R_{free} test set	2851 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtrriage
Anisotropy	0.529	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11419	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: EDO

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	0.89	0/2756	0.92	3/3761 (0.1%)
1	B	0.85	2/2756 (0.1%)	0.90	3/3761 (0.1%)
1	C	0.90	0/2756	0.93	3/3761 (0.1%)
1	D	0.91	2/2756 (0.1%)	0.91	0/3761
All	All	0.89	4/11024 (0.0%)	0.92	9/15044 (0.1%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	LYS	CA-C	5.88	1.59	1.53
1	D	206	LEU	CA-C	-5.52	1.45	1.52
1	D	238	LYS	CA-C	5.45	1.59	1.53
1	B	306	ARG	CA-C	-5.08	1.47	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ILE	CG1-CB-CG2	-8.47	85.28	110.70
1	C	4	ARG	CA-C-N	-6.94	112.64	119.78
1	C	4	ARG	C-N-CA	-6.94	112.64	119.78
1	B	4	ARG	CA-C-N	-6.30	113.29	119.78
1	B	4	ARG	C-N-CA	-6.30	113.29	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	VAL	CB-CA-C	-5.55	104.24	110.96
1	A	4	ARG	CA-C-N	-5.54	114.07	119.78
1	A	4	ARG	C-N-CA	-5.54	114.07	119.78
1	A	238	LYS	CB-CA-C	-5.31	103.97	112.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	GLY	Peptide

5.2 Too-close contacts [i](#)

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	2699	0	2724	21	0
1	B	2699	0	2724	24	0
1	C	2699	0	2724	24	0
1	D	2699	0	2724	38	0
2	A	4	0	6	0	0
3	A	198	0	0	9	0
3	B	122	0	0	8	0
3	C	168	0	0	10	0
3	D	131	0	0	23	0
All	All	11419	0	10902	94	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 4.

All (94) 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:D:189:ALA:CA	3:D:405:HOH:O	2.14	0.94
1:D:189:ALA:HA	3:D:405:HOH:O	1.67	0.93
1:A:189:ALA:N	3:A:501:HOH:O	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LYS:HE3	3:D:419:HOH:O	1.72	0.90
1:C:4:ARG:HD3	3:C:414:HOH:O	1.69	0.90
1:C:296:GLN:HG3	3:C:527:HOH:O	1.71	0.90
1:D:42:ARG:HD3	3:D:457:HOH:O	1.73	0.88
1:B:200:MET:CE	1:D:252:ILE:HG13	2.05	0.87
1:B:253:ASP:HB3	3:B:454:HOH:O	1.75	0.84
1:B:200:MET:HE3	1:D:252:ILE:HG13	1.60	0.83
1:A:114:ASN:HB3	3:A:527:HOH:O	1.82	0.80
1:B:189:ALA:HB2	3:B:514:HOH:O	1.83	0.77
1:D:296:GLN:HG3	3:D:509:HOH:O	1.84	0.77
1:A:146:LYS:HD2	3:A:691:HOH:O	1.89	0.72
1:D:362:GLY:HA2	3:D:404:HOH:O	1.89	0.72
1:B:56:LEU:HB3	3:B:401:HOH:O	1.90	0.72
1:D:39:ALA:HB3	1:D:69:VAL:HG11	1.75	0.67
1:D:189:ALA:HB2	3:D:525:HOH:O	1.94	0.66
1:A:189:ALA:CA	3:A:501:HOH:O	2.42	0.66
1:A:361:LYS:HE2	3:A:671:HOH:O	1.95	0.65
1:D:313:LYS:HD3	3:D:485:HOH:O	1.97	0.65
1:D:198:ASP:OD2	3:D:401:HOH:O	2.15	0.65
1:D:313:LYS:HB3	3:D:474:HOH:O	1.99	0.62
1:B:63:ALA:HB2	3:B:512:HOH:O	2.01	0.60
1:C:62:ASP:OD1	1:C:65:ARG:NH2	2.32	0.59
1:A:189:ALA:HA	3:A:501:HOH:O	2.00	0.58
1:C:68:VAL:HG12	3:C:498:HOH:O	2.03	0.57
1:D:193:GLY:N	3:D:406:HOH:O	2.38	0.56
1:D:189:ALA:N	3:D:405:HOH:O	2.33	0.56
1:C:193:GLY:N	3:C:406:HOH:O	2.39	0.56
1:D:217:GLU:OE1	3:D:402:HOH:O	2.18	0.55
1:D:73:ARG:NH2	3:D:407:HOH:O	2.38	0.55
1:C:296:GLN:CG	3:C:527:HOH:O	2.39	0.55
1:C:313:LYS:HB3	3:C:462:HOH:O	2.06	0.54
1:C:365:GLN:CB	3:C:557:HOH:O	2.55	0.54
1:B:296:GLN:HG3	3:B:497:HOH:O	2.07	0.54
1:D:4:ARG:HA	3:D:486:HOH:O	2.09	0.53
1:B:310:ARG:HD2	1:C:252:ILE:HD13	1.90	0.53
1:A:250:PRO:HA	1:C:200:MET:HE1	1.90	0.53
1:D:189:ALA:C	3:D:405:HOH:O	2.46	0.53
1:A:208:SER:HB3	3:A:660:HOH:O	2.09	0.52
1:A:197:LEU:HG	1:C:186:ILE:CD1	2.39	0.52
1:C:236:ALA:HB1	1:C:237:PRO:HA	1.93	0.51
1:A:296:GLN:HG3	3:A:625:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:HB1	1:B:237:PRO:HA	1.93	0.49
1:D:236:ALA:HB1	1:D:237:PRO:HA	1.93	0.48
1:D:120:LEU:HD12	3:D:423:HOH:O	2.13	0.48
1:D:362:GLY:CA	3:D:404:HOH:O	2.56	0.48
1:D:42:ARG:O	1:D:42:ARG:NH1	2.44	0.48
1:C:42:ARG:O	1:C:42:ARG:NH1	2.45	0.47
1:B:223:GLY:C	3:B:444:HOH:O	2.56	0.47
1:C:365:GLN:HB2	3:C:557:HOH:O	2.14	0.47
1:D:163:VAL:HB	1:D:164:PRO:HD3	1.97	0.47
1:A:163:VAL:HB	1:A:164:PRO:HD3	1.97	0.47
1:B:200:MET:CE	1:D:252:ILE:CG1	2.87	0.46
1:A:236:ALA:HB1	1:A:237:PRO:HA	1.97	0.46
1:C:4:ARG:NH1	3:C:414:HOH:O	2.49	0.46
1:C:285:ALA:HB2	1:C:357:ILE:HD11	1.98	0.46
1:A:262:LYS:HD3	3:A:629:HOH:O	2.15	0.46
1:B:63:ALA:CB	3:B:512:HOH:O	2.62	0.46
1:C:163:VAL:HB	1:C:164:PRO:HD3	1.97	0.46
1:D:313:LYS:CD	3:D:485:HOH:O	2.60	0.46
1:D:253:ASP:HB2	3:D:485:HOH:O	2.16	0.45
1:D:313:LYS:CE	3:D:440:HOH:O	2.63	0.45
1:D:182:THR:C	1:D:183:LEU:HD12	2.42	0.45
1:A:285:ALA:HB2	1:A:357:ILE:HD11	1.99	0.45
1:D:285:ALA:HB2	1:D:357:ILE:HD11	1.99	0.45
1:A:197:LEU:HG	1:C:186:ILE:HD12	1.98	0.44
1:D:156:CYS:SG	3:D:520:HOH:O	2.34	0.44
1:B:163:VAL:HB	1:B:164:PRO:HD3	1.98	0.44
1:A:250:PRO:CA	1:C:200:MET:HE1	2.47	0.44
1:A:182:THR:C	1:A:183:LEU:HD12	2.43	0.44
1:C:182:THR:C	1:C:183:LEU:HD12	2.43	0.44
1:B:285:ALA:HB2	1:B:357:ILE:HD11	1.99	0.43
1:C:153:ASN:HB2	3:C:438:HOH:O	2.19	0.43
1:B:186:ILE:CD1	1:D:197:LEU:HG	2.48	0.43
1:D:238:LYS:HG3	3:D:522:HOH:O	2.18	0.43
1:A:179:ILE:HD12	1:B:179:ILE:HD12	2.01	0.43
1:D:9:VAL:HG12	1:D:84:VAL:HG13	2.01	0.43
1:B:186:ILE:HD12	1:D:197:LEU:HG	2.00	0.43
1:B:200:MET:HG2	1:D:200:MET:SD	2.59	0.42
1:A:153:ASN:OD1	1:A:350:SER:HB3	2.19	0.42
1:A:241:ASN:HB3	1:B:331:VAL:HG22	2.01	0.42
1:C:129:ASN:N	1:C:130:PRO:CD	2.82	0.42
1:B:365:GLN:NE2	3:B:403:HOH:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASN:OD1	1:B:350:SER:HB3	2.20	0.41
1:C:4:ARG:HB2	1:C:5:PRO:HD3	2.02	0.41
1:B:182:THR:C	1:B:183:LEU:HD12	2.45	0.41
1:B:4:ARG:HB2	1:B:5:PRO:HD3	2.03	0.41
1:A:187:SER:O	1:A:188:GLY:C	2.64	0.40
1:D:129:ASN:N	1:D:130:PRO:CD	2.84	0.40
1:C:65:ARG:HD3	1:C:66:HIS:NE2	2.37	0.40
1:D:39:ALA:HB3	1:D:69:VAL:CG1	2.46	0.40
1:B:64:VAL:O	1:B:65:ARG:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	355/375 (95%)	344 (97%)	10 (3%)	1 (0%)	36	58
1	B	355/375 (95%)	346 (98%)	9 (2%)	0	100	100
1	C	355/375 (95%)	344 (97%)	10 (3%)	1 (0%)	36	58
1	D	355/375 (95%)	343 (97%)	11 (3%)	1 (0%)	36	58
All	All	1420/1500 (95%)	1377 (97%)	40 (3%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLY
1	D	188	GLY
1	C	188	GLY

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	294/308 (96%)	283 (96%)	11 (4%)	30	57
1	B	294/308 (96%)	287 (98%)	7 (2%)	43	70
1	C	294/308 (96%)	284 (97%)	10 (3%)	32	60
1	D	294/308 (96%)	286 (97%)	8 (3%)	39	67
All	All	1176/1232 (96%)	1140 (97%)	36 (3%)	35	63

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	73	ARG
1	A	113	LYS
1	A	146	LYS
1	A	194	VAL
1	A	196	SER
1	A	238	LYS
1	A	262	LYS
1	A	266	SER
1	A	311	LEU
1	A	344	ARG
1	B	55	LYS
1	B	73	ARG
1	B	113	LYS
1	B	146	LYS
1	B	262	LYS
1	B	266	SER
1	B	344	ARG
1	C	17	THR
1	C	50	ARG
1	C	55	LYS
1	C	73	ARG
1	C	146	LYS
1	C	238	LYS

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Mol	Chain	Res	Type
1	C	266	SER
1	C	311	LEU
1	C	334	ILE
1	C	344	ARG
1	D	50	ARG
1	D	55	LYS
1	D	71	GLU
1	D	73	ARG
1	D	146	LYS
1	D	262	LYS
1	D	266	SER
1	D	344	ARG

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	46	GLN
1	A	184	GLN
1	A	239	GLN
1	A	241	ASN
1	B	46	GLN
1	B	184	GLN
1	B	241	ASN
1	C	6	GLN
1	C	70	HIS
1	C	184	GLN
1	D	46	GLN
1	D	70	HIS
1	D	184	GLN
1	D	241	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](#)

1 ligand is 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	EDO	A	401	-	3,3,3	0.51	0	2,2,2	0.62	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	EDO	A	401	-	-	1/1/1/1	-

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	401	EDO	O1-C1-C2-O2

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/375 (95%)	-0.39	3 (0%) 82 80	22, 35, 62, 92	0
1	B	359/375 (95%)	-0.03	9 (2%) 58 52	22, 45, 76, 99	0
1	C	359/375 (95%)	-0.23	5 (1%) 73 69	22, 37, 76, 107	0
1	D	359/375 (95%)	0.24	14 (3%) 43 38	23, 48, 85, 133	0
All	All	1436/1500 (95%)	-0.10	31 (2%) 62 57	22, 41, 77, 133	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	57	PRO	3.6
1	D	50	ARG	3.3
1	C	63	ALA	3.2
1	C	55	LYS	2.9
1	D	343	VAL	2.8
1	B	64	VAL	2.8
1	D	365	GLN	2.7
1	A	365	GLN	2.7
1	C	189	ALA	2.7
1	D	320	CYS	2.6
1	C	50	ARG	2.6
1	B	58	SER	2.5
1	B	63	ALA	2.4
1	B	189	ALA	2.4
1	B	316	HIS	2.4
1	D	316	HIS	2.3
1	B	113	LYS	2.3
1	A	189	ALA	2.3
1	B	146	LYS	2.2
1	D	189	ALA	2.2
1	B	365	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	315	LEU	2.2
1	D	364	ILE	2.2
1	B	4	ARG	2.2
1	D	111	ASN	2.1
1	D	63	ALA	2.1
1	D	319	ALA	2.1
1	D	147	LYS	2.1
1	A	188	GLY	2.0
1	D	146	LYS	2.0
1	D	5	PRO	2.0

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	EDO	A	401	4/4	0.98	0.11	45,47,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.