Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2021 – 06:45 PM EST

PDB ID	:	3K9D
Title	:	CRYSTAL STRUCTURE OF PROBABLE ALDEHYDE DEHYDROGENASE FROM Listeria monocytogenes EGD-e
Authors	:	Patskovsky, Y.; Toro, R.; Freeman, J.; Miller, S.; Sauder, J.M.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-10-15
Resolution	:	2.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

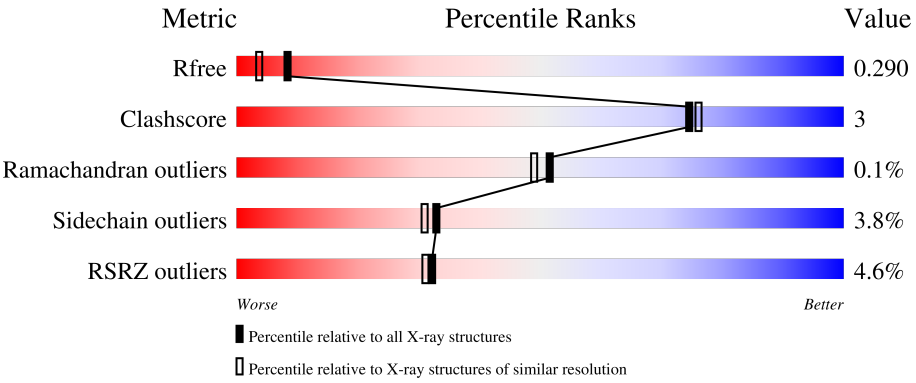
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	464	90% 7%
1	B	464	2% 87% 10%
1	C	464	91% 6%
1	D	464	16% 86% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14136 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	2	0
			3409	2154	591	649	15			
1	B	454	Total	C	N	O	S	0	3	0
			3414	2158	592	649	15			
1	C	454	Total	C	N	O	S	0	4	0
			3422	2161	594	651	16			
1	D	453	Total	C	N	O	S	0	2	0
			3406	2149	593	649	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8Y7U1
A	2	SER	-	expression tag	UNP Q8Y7U1
A	457	GLU	-	expression tag	UNP Q8Y7U1
A	458	GLY	-	expression tag	UNP Q8Y7U1
A	459	HIS	-	expression tag	UNP Q8Y7U1
A	460	HIS	-	expression tag	UNP Q8Y7U1
A	461	HIS	-	expression tag	UNP Q8Y7U1
A	462	HIS	-	expression tag	UNP Q8Y7U1
A	463	HIS	-	expression tag	UNP Q8Y7U1
A	464	HIS	-	expression tag	UNP Q8Y7U1
B	1	MET	-	expression tag	UNP Q8Y7U1
B	2	SER	-	expression tag	UNP Q8Y7U1
B	457	GLU	-	expression tag	UNP Q8Y7U1
B	458	GLY	-	expression tag	UNP Q8Y7U1
B	459	HIS	-	expression tag	UNP Q8Y7U1
B	460	HIS	-	expression tag	UNP Q8Y7U1
B	461	HIS	-	expression tag	UNP Q8Y7U1
B	462	HIS	-	expression tag	UNP Q8Y7U1
B	463	HIS	-	expression tag	UNP Q8Y7U1
B	464	HIS	-	expression tag	UNP Q8Y7U1
C	1	MET	-	expression tag	UNP Q8Y7U1

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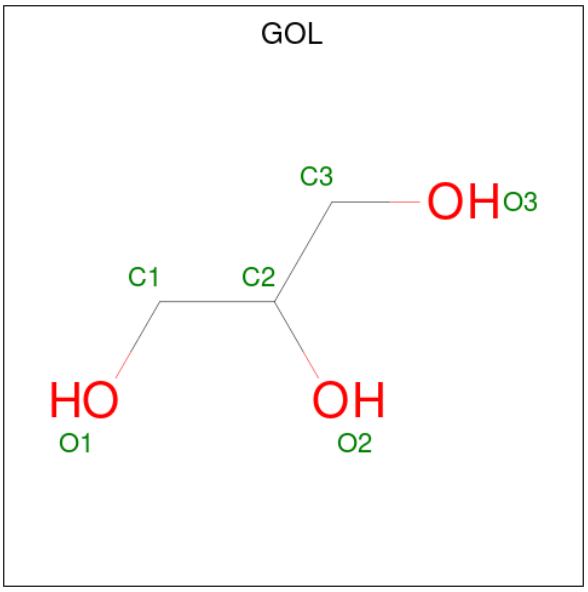
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	SER	-	expression tag	UNP Q8Y7U1
C	457	GLU	-	expression tag	UNP Q8Y7U1
C	458	GLY	-	expression tag	UNP Q8Y7U1
C	459	HIS	-	expression tag	UNP Q8Y7U1
C	460	HIS	-	expression tag	UNP Q8Y7U1
C	461	HIS	-	expression tag	UNP Q8Y7U1
C	462	HIS	-	expression tag	UNP Q8Y7U1
C	463	HIS	-	expression tag	UNP Q8Y7U1
C	464	HIS	-	expression tag	UNP Q8Y7U1
D	1	MET	-	expression tag	UNP Q8Y7U1
D	2	SER	-	expression tag	UNP Q8Y7U1
D	457	GLU	-	expression tag	UNP Q8Y7U1
D	458	GLY	-	expression tag	UNP Q8Y7U1
D	459	HIS	-	expression tag	UNP Q8Y7U1
D	460	HIS	-	expression tag	UNP Q8Y7U1
D	461	HIS	-	expression tag	UNP Q8Y7U1
D	462	HIS	-	expression tag	UNP Q8Y7U1
D	463	HIS	-	expression tag	UNP Q8Y7U1
D	464	HIS	-	expression tag	UNP Q8Y7U1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

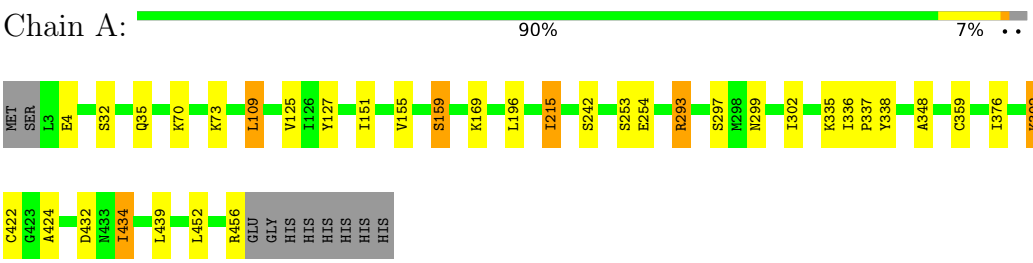
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	204	Total O 204 204	0	0
4	B	78	Total O 78 78	0	0
4	C	162	Total O 162 162	0	0
4	D	32	Total O 32 32	0	0

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.

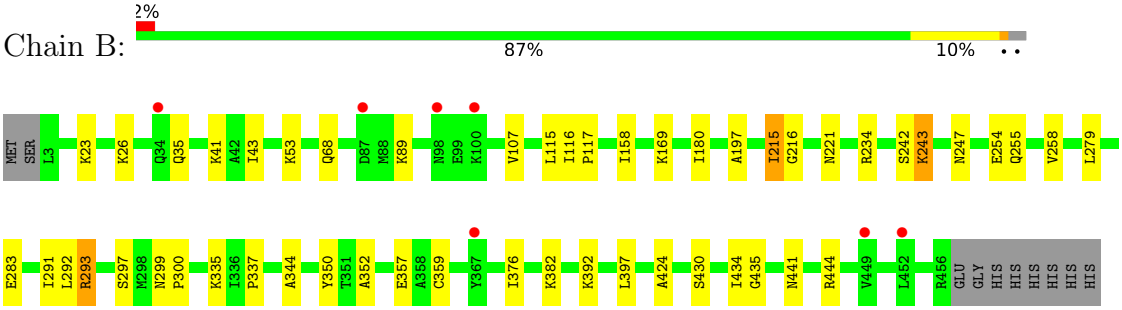
• Molecule 1: ALDEHYDE DEHYDROGENASE

Chain A:



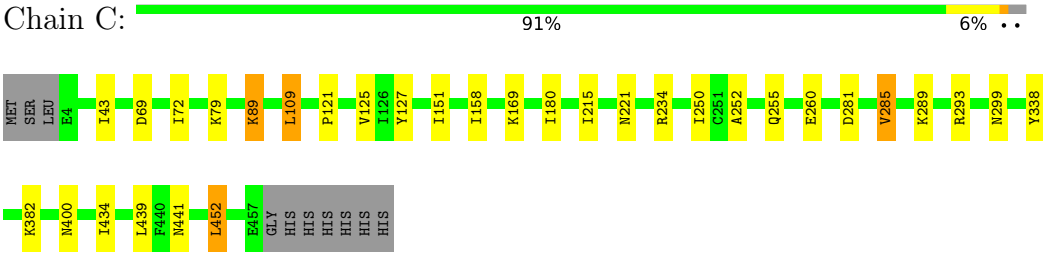
• Molecule 1: ALDEHYDE DEHYDROGENASE

Chain B:



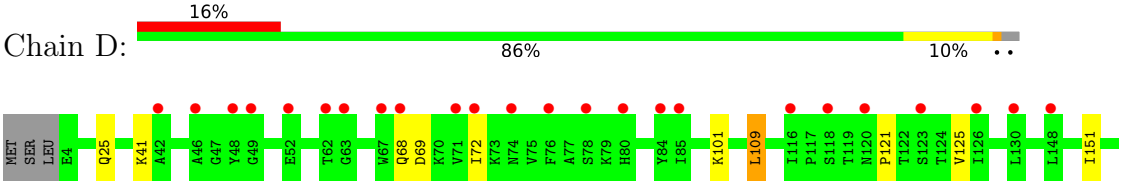
• Molecule 1: ALDEHYDE DEHYDROGENASE

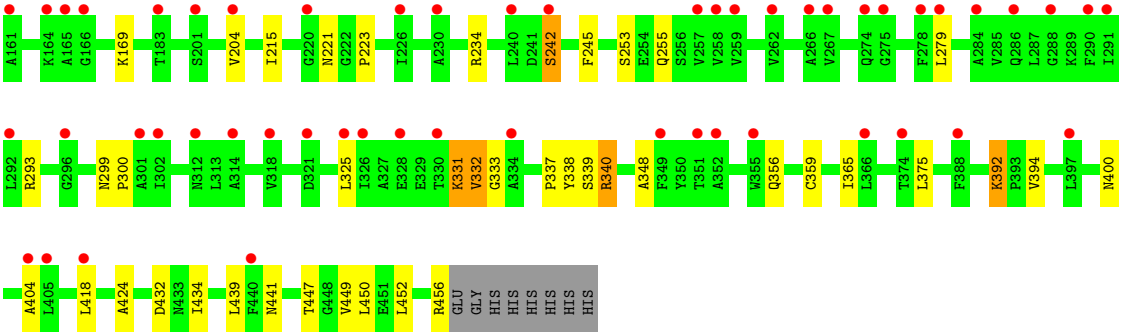
Chain C:



• Molecule 1: ALDEHYDE DEHYDROGENASE

Chain D:




A161 K164 A165 G166 K169 T183 S201 V204 I215 G220 N221 G222 P223 I226 A230 R234 L240 D241 S242 F245 S253 E254 Q255 S256 V257 V258 V259 V262 A266 V267 Q274 G275 F278 L279 A284 V285 Q286 L287 G288 K289 F290 I291
L292 R293 G296 N299 P300 A301 I302 N312 L313 A314 V318 D321 L325 I326 A327 E328 E329 T330 K331 V332 G333 A334 P337 Y338 S339 R340 A348 F349 Y350 T351 A352 W355 Q356 C359 I365 L366 T374 L375 F388 K392 P393 V394 L397 M400
A404 L405 L418 A424 D432 N433 I434 L439 F440 N441 T447 G448 V449 L450 E451 L452 R456 GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	226.09Å 226.09Å 81.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 45.57 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.4 (45.57-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.239 , 0.292 0.239 , 0.290	Depositor DCC
R_{free} test set	5122 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 19.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.076 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14136	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CL

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	0.50	0/3467	0.63	0/4693
1	B	0.43	0/3475	0.60	0/4702
1	C	0.49	0/3486	0.64	0/4716
1	D	0.44	0/3463	0.59	0/4684
All	All	0.46	0/13891	0.62	0/18795

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	332	VAL	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	3409	0	3521	20	0
1	B	3414	0	3532	24	0
1	C	3422	0	3537	18	0
1	D	3406	0	3511	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	C	6	0	8	0	0
4	A	204	0	0	1	0
4	B	78	0	0	1	0
4	C	162	0	0	0	0
4	D	32	0	0	1	0
All	All	14136	0	14109	90	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 3.

All (90) 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:215:ILE:HD11	1:A:434:ILE:HG21	1.57	0.84
1:D:332:VAL:HG12	1:D:333:GLY:CA	2.16	0.75
1:D:215:ILE:HD11	1:D:434:ILE:HD12	1.68	0.74
1:D:234:ARG:HH12	1:D:400:ASN:HB3	1.55	0.72
1:D:332:VAL:HG13	1:D:339:SER:HB2	1.77	0.67
1:D:332:VAL:HG12	1:D:333:GLY:N	2.11	0.66
1:B:215:ILE:HD11	1:B:434:ILE:HD11	1.79	0.65
1:A:215:ILE:CD1	1:A:434:ILE:HG21	2.25	0.64
1:B:441:ASN:HD21	1:D:424:ALA:H	1.44	0.63
1:A:405:LEU:HD21	1:C:452:LEU:HG	1.82	0.61
1:A:32:SER:H	1:A:35:GLN:HE21	1.49	0.61
1:A:155:VAL:O	1:A:159:SER:HB2	2.00	0.60
1:D:359:CYS:SG	1:D:392:LYS:NZ	2.74	0.60
1:B:43:ILE:HG23	1:B:158:ILE:HB	1.83	0.60
1:B:424:ALA:H	1:D:441:ASN:HD21	1.50	0.58
1:B:254:GLU:HG3	1:B:376:ILE:HD13	1.86	0.57
1:A:424:ALA:H	1:C:441:ASN:HD21	1.51	0.57
1:A:254:GLU:HG3	1:A:376:ILE:HD13	1.85	0.57
1:B:115:LEU:HD12	1:B:197:ALA:HA	1.87	0.56
1:D:101:LYS:HB3	1:D:447:THR:HB	1.89	0.54
1:B:292:LEU:HB2	1:B:337:PRO:HG3	1.89	0.54
1:B:23:LYS:HA	1:B:26:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG21	1:A:151:ILE:HG23	1.89	0.54
1:C:215:ILE:HD11	1:C:434:ILE:CD1	2.38	0.53
1:D:333:GLY:HA2	1:D:339:SER:OG	2.09	0.53
1:D:337:PRO:HA	1:D:340:ARG:HG3	1.90	0.53
1:B:247:ASN:ND2	4:B:523:HOH:O	2.32	0.52
1:C:215:ILE:HD11	1:C:434:ILE:HD12	1.89	0.52
1:D:69[B]:ASP:HB2	1:D:245:PHE:CE1	2.45	0.52
1:B:243[B]:LYS:HE3	1:B:344:ALA:O	2.10	0.52
1:B:279:LEU:HB3	1:B:283:GLU:HG3	1.93	0.51
1:B:215:ILE:HD13	1:B:430:SER:HB3	1.93	0.51
1:C:43:ILE:HG23	1:C:158:ILE:HB	1.93	0.50
1:C:89:LYS:HE3	1:C:89:LYS:HA	1.93	0.50
1:C:338:TYR:HB3	1:C:348:ALA:HB2	1.92	0.50
1:C:293:ARG:HD2	1:C:299:ASN:HA	1.94	0.50
1:D:221:ASN:HA	1:D:255:GLN:HG3	1.93	0.49
1:D:279:LEU:HD21	1:D:325:LEU:HD22	1.94	0.49
1:A:338:TYR:HB3	1:A:348:ALA:HB2	1.93	0.49
1:D:332:VAL:HG13	1:D:339:SER:CB	2.43	0.48
1:D:255:GLN:HB3	4:D:488:HOH:O	2.13	0.48
1:C:125:VAL:HG21	1:C:151:ILE:HG23	1.96	0.47
1:D:338:TYR:HB3	1:D:348:ALA:HB2	1.96	0.47
1:A:253:SER:HB3	1:A:404:ALA:HB2	1.96	0.47
1:B:197:ALA:HB3	1:B:216:GLY:HA2	1.96	0.47
1:A:109:LEU:HD22	1:A:439:LEU:HA	1.96	0.47
1:B:352:ALA:HB1	1:B:357:GLU:HB3	1.97	0.47
1:B:221:ASN:HA	1:B:255:GLN:HG3	1.96	0.47
1:D:221:ASN:ND2	1:D:339:SER:O	2.47	0.47
1:D:375:LEU:HD22	1:D:392:LYS:HG2	1.96	0.47
1:B:434:ILE:HG22	1:B:435:GLY:N	2.29	0.45
1:D:253:SER:HB3	1:D:404:ALA:HB2	1.97	0.45
1:D:242:SER:HB2	1:D:404:ALA:H	1.82	0.45
1:A:422:CYS:HB3	4:A:530:HOH:O	2.16	0.45
1:B:293:ARG:NH2	1:B:297[B]:SER:OG	2.51	0.44
1:A:32:SER:H	1:A:35:GLN:NE2	2.12	0.44
1:B:243[B]:LYS:HA	1:B:243[B]:LYS:HD2	1.71	0.44
1:D:332:VAL:HG12	1:D:333:GLY:HA3	1.95	0.44
1:C:89:LYS:HE3	1:C:89:LYS:CA	2.44	0.44
1:B:392:LYS:HA	1:B:392:LYS:HD3	1.81	0.43
1:B:258:VAL:HG22	1:B:350:TYR:HB2	2.00	0.43
1:D:215:ILE:HD11	1:D:434:ILE:CD1	2.44	0.43
1:D:392:LYS:HB3	1:D:394:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HA	1:A:73:LYS:HD3	2.01	0.42
1:C:121:PRO:O	1:C:125:VAL:HG23	2.19	0.42
1:D:331:LYS:HA	1:D:331:LYS:HD2	1.30	0.42
1:B:107:VAL:HB	1:B:441:ASN:HB2	2.01	0.42
1:A:432:ASP:HB2	1:A:434:ILE:HG22	2.01	0.42
1:B:444:ARG:NH2	1:D:432:ASP:OD1	2.51	0.42
1:D:109:LEU:HD22	1:D:439:LEU:HA	2.01	0.42
1:C:281:ASP:O	1:C:285:VAL:HG12	2.19	0.42
1:C:109:LEU:HD22	1:C:439:LEU:HA	2.01	0.42
1:C:221:ASN:HA	1:C:255:GLN:HG3	2.01	0.42
1:D:125:VAL:HG21	1:D:151:ILE:HG23	2.02	0.42
1:D:69[A]:ASP:HA	1:D:72:ILE:HD12	2.00	0.42
1:A:299:ASN:O	1:A:302:ILE:HG12	2.20	0.42
1:A:336:ILE:HA	1:A:337:PRO:HD2	1.95	0.42
1:C:250:ILE:HG22	1:C:252:ALA:H	1.84	0.42
1:B:116:ILE:HA	1:B:117:PRO:HD3	1.93	0.41
1:C:234:ARG:HH12	1:C:400:ASN:HB3	1.85	0.41
1:A:293:ARG:NH2	1:A:297:SER:OG	2.53	0.41
1:C:260:GLU:HA	1:C:352:ALA:O	2.20	0.41
1:A:196:LEU:HD23	1:A:215:ILE:HG23	2.03	0.41
1:C:69:ASP:HA	1:C:72:ILE:HD12	2.03	0.41
1:D:299:ASN:HA	1:D:300:PRO:HD3	1.89	0.41
1:D:223:PRO:HD2	1:D:375:LEU:HD12	2.03	0.41
1:B:299:ASN:HA	1:B:300:PRO:HD3	1.92	0.40
1:A:359:CYS:SG	1:A:392:LYS:NZ	2.79	0.40
1:D:449:VAL:HG12	1:D:450:LEU:HG	2.03	0.40
1:D:332:VAL:HG11	1:D:365:ILE:HA	2.04	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	454/464 (98%)	449 (99%)	5 (1%)	0	100	100
1	B	455/464 (98%)	445 (98%)	10 (2%)	0	100	100
1	C	456/464 (98%)	449 (98%)	7 (2%)	0	100	100
1	D	452/464 (97%)	433 (96%)	18 (4%)	1 (0%)	47	44
All	All	1817/1856 (98%)	1776 (98%)	40 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	121	PRO

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	366/373 (98%)	353 (96%)	13 (4%)	35	34
1	B	367/373 (98%)	349 (95%)	18 (5%)	25	21
1	C	368/373 (99%)	357 (97%)	11 (3%)	41	41
1	D	365/373 (98%)	349 (96%)	16 (4%)	28	25
All	All	1466/1492 (98%)	1408 (96%)	58 (4%)	33	29

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	109	LEU
1	A	127	TYR
1	A	159	SER
1	A	169	LYS
1	A	215	ILE
1	A	242	SER
1	A	293	ARG
1	A	335	LYS
1	A	392	LYS

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Mol	Chain	Res	Type
1	A	434	ILE
1	A	452	LEU
1	A	456	ARG
1	B	35	GLN
1	B	41	LYS
1	B	53	LYS
1	B	68	GLN
1	B	89	LYS
1	B	169	LYS
1	B	180	ILE
1	B	215	ILE
1	B	234	ARG
1	B	242	SER
1	B	243[A]	LYS
1	B	243[B]	LYS
1	B	291	ILE
1	B	293	ARG
1	B	335	LYS
1	B	359	CYS
1	B	382	LYS
1	B	397	LEU
1	C	79[A]	LYS
1	C	79[B]	LYS
1	C	89	LYS
1	C	109	LEU
1	C	127	TYR
1	C	169	LYS
1	C	180	ILE
1	C	285	VAL
1	C	289	LYS
1	C	382	LYS
1	C	452	LEU
1	D	25	GLN
1	D	41	LYS
1	D	68	GLN
1	D	109	LEU
1	D	169	LYS
1	D	204	VAL
1	D	242	SER
1	D	293	ARG
1	D	331	LYS
1	D	340	ARG

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Mol	Chain	Res	Type
1	D	356	GLN
1	D	392	LYS
1	D	418	LEU
1	D	452	LEU
1	D	456[A]	ARG
1	D	456[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	286	GLN
1	B	25	GLN
1	B	286	GLN
1	B	373	HIS
1	B	441	ASN
1	C	441	ASN
1	D	25	GLN
1	D	356	GLN
1	D	441	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	GOL	C	466	-	5,5,5	0.20	0	5,5,5	0.92	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
3	GOL	C	466	-	-	1/4/4/4	-

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
3	C	466	GOL	C1-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

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, 95^{th} 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	454/464 (97%)	-0.11	0 100 100	10, 20, 31, 40	0
1	B	454/464 (97%)	0.21	7 (1%) 73 72	11, 20, 31, 39	0
1	C	454/464 (97%)	-0.08	0 100 100	11, 20, 31, 50	0
1	D	453/464 (97%)	1.07	76 (16%) 1 1	11, 20, 31, 40	0
All	All	1815/1856 (97%)	0.27	83 (4%) 32 31	10, 20, 31, 50	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	TYR	7.7
1	D	267	VAL	7.3
1	D	291	ILE	5.9
1	D	355	TRP	5.8
1	D	302	ILE	5.5
1	D	292	LEU	5.3
1	D	284	ALA	5.1
1	D	301	ALA	4.9
1	D	352	ALA	4.6
1	D	290	PHE	4.4
1	D	242	SER	4.3
1	D	405	LEU	4.2
1	D	259	VAL	4.1
1	D	288	GLY	4.1
1	D	48	TYR	4.0
1	D	296	GLY	4.0
1	D	165	ALA	3.8
1	B	449	VAL	3.8
1	D	118	SER	3.8
1	D	78	SER	3.6
1	D	257	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	325	LEU	3.4
1	D	388	PHE	3.3
1	D	126	ILE	3.3
1	D	321	ASP	3.3
1	D	76	PHE	3.3
1	D	130	LEU	3.3
1	B	98	ASN	3.3
1	D	278	PHE	3.2
1	B	367	TYR	3.1
1	D	266	ALA	3.1
1	B	452	LEU	3.0
1	D	349	PHE	3.0
1	B	34	GLN	3.0
1	D	366	LEU	2.9
1	D	52	GLU	2.9
1	D	46	ALA	2.8
1	D	183	THR	2.8
1	D	418	LEU	2.8
1	D	220	GLY	2.8
1	D	279	LEU	2.8
1	D	63	GLY	2.7
1	D	397	LEU	2.7
1	D	67	TRP	2.7
1	D	374	THR	2.7
1	D	440	PHE	2.7
1	D	351	THR	2.6
1	D	120	ASN	2.6
1	D	230	ALA	2.6
1	D	201	SER	2.6
1	D	312	ASN	2.6
1	D	318	VAL	2.5
1	D	74	ASN	2.5
1	D	326	ILE	2.5
1	D	68	GLN	2.5
1	D	49	GLY	2.5
1	D	240	LEU	2.5
1	D	328	GLU	2.5
1	D	334	ALA	2.5
1	D	71	VAL	2.4
1	D	286	GLN	2.4
1	B	87	ASP	2.4
1	D	72	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	100	LYS	2.4
1	D	275	GLY	2.4
1	D	166	GLY	2.3
1	D	80	HIS	2.3
1	D	258	VAL	2.3
1	D	404	ALA	2.3
1	D	123	SER	2.2
1	D	62	THR	2.2
1	D	161	ALA	2.2
1	D	226	ILE	2.2
1	D	274	GLN	2.2
1	D	148	LEU	2.2
1	D	262	VAL	2.1
1	D	164	LYS	2.1
1	D	330	THR	2.1
1	D	204	VAL	2.0
1	D	314	ALA	2.0
1	D	116	ILE	2.0
1	D	42	ALA	2.0
1	D	85	ILE	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 monosaccharides 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, 95^{th} 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
3	GOL	C	466	6/6	0.88	0.20	6,20,31,31	0
2	CL	C	465	1/1	0.95	0.18	46,46,46,46	0
2	CL	B	465	1/1	0.96	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	A	465	1/1	0.98	0.05	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.