



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:36 PM UTC

PDB ID : 7CAZ / pdb_00007caz
Title : Crystal structure of bacterial reductase
Authors : Kim, Y.; Lee, W.C.
Deposited on : 2020-06-10
Resolution : 1.79 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

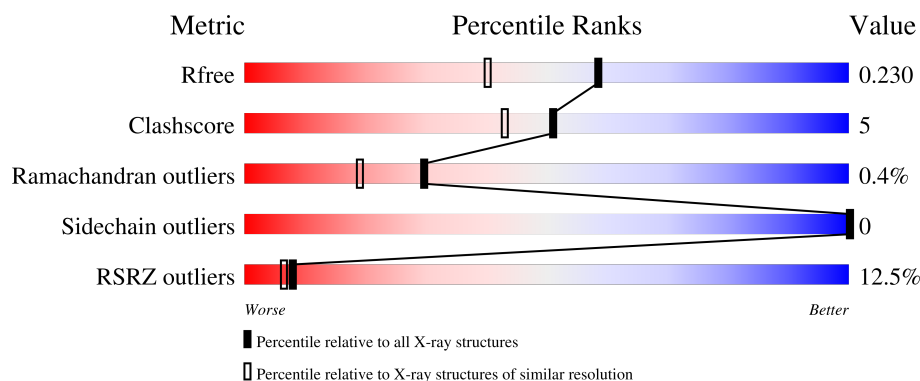
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	244	12% 86% 11% ..
1	B	244	13% 87% 10% ..
1	C	244	13% 90% 8% ..
1	D	244	11% 88% 9% ..

2 Entry composition [i](#)

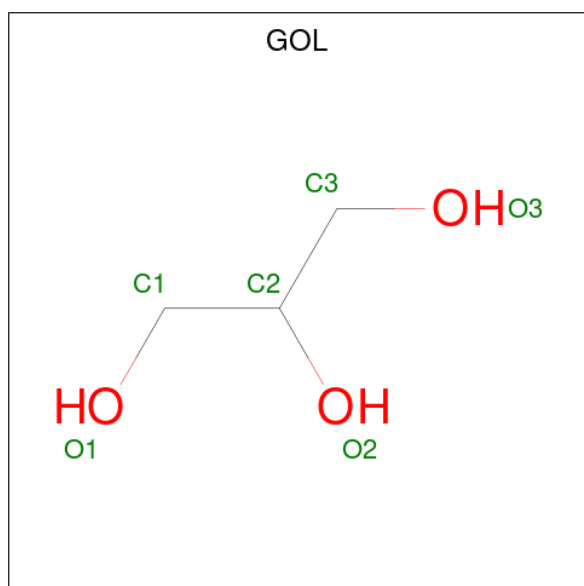
There are 3 unique types of molecules in this entry. The entry contains 7766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1800	1125	320	349	6			
1	B	240	Total	C	N	O	S	0	1	0
			1806	1129	320	351	6			
1	C	242	Total	C	N	O	S	0	1	0
			1824	1139	323	356	6			
1	D	240	Total	C	N	O	S	0	1	0
			1803	1127	320	350	6			

- 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		

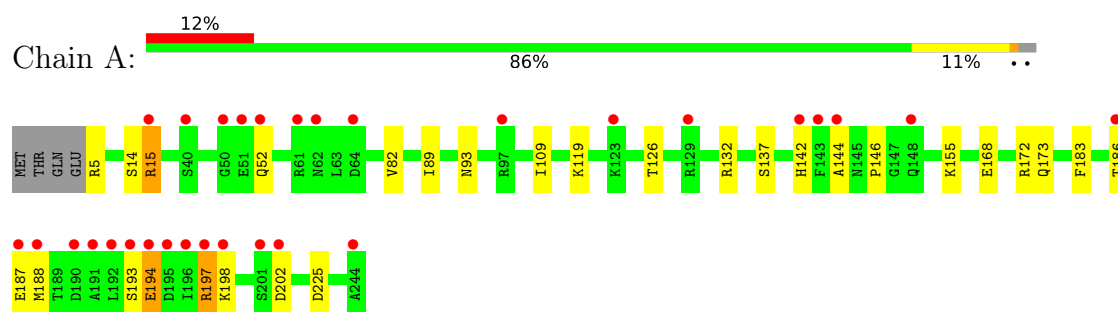
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total 134	O 134	0	0
3	B	138	Total 138	O 138	0	0
3	C	121	Total 121	O 121	0	0
3	D	134	Total 134	O 134	0	0

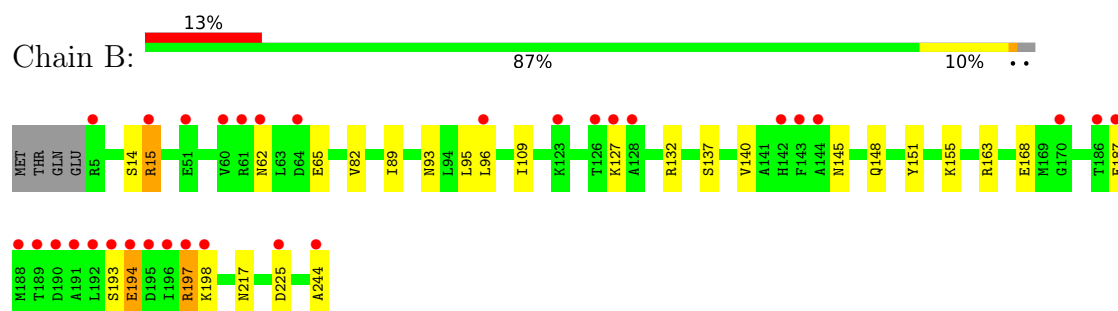
3 Residue-property plots [i](#)

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.

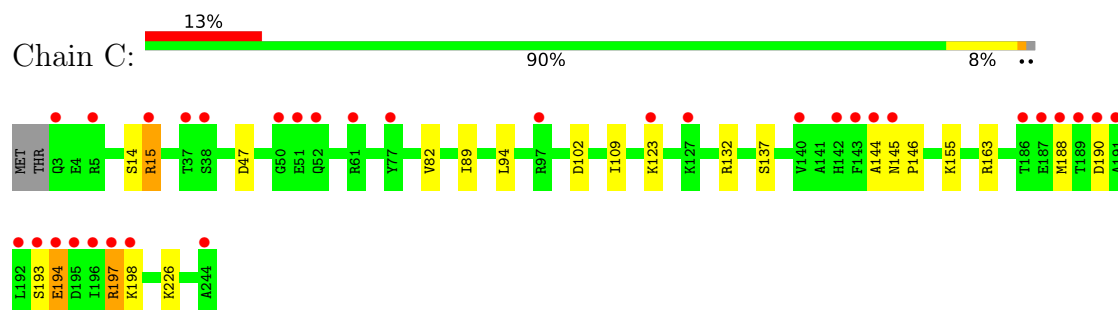
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



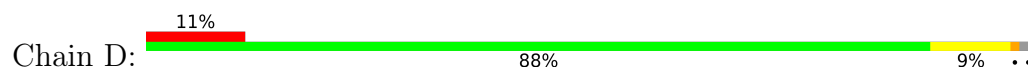
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

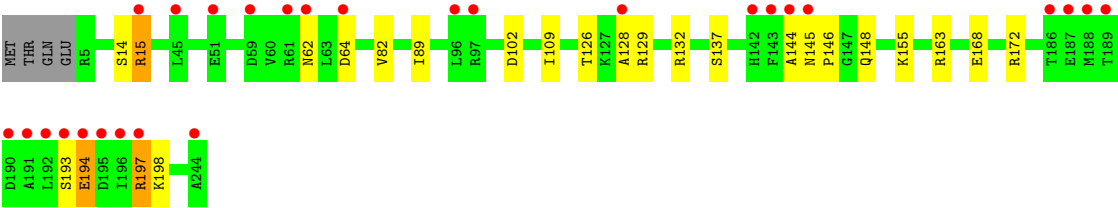


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.61Å 100.04Å 120.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.79 19.91 – 1.79	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.91-1.79) 88.4 (19.91-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.11 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.207 , 0.229 0.207 , 0.230	Depositor DCC
R_{free} test set	1929 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7766	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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	0.43	0/1822	0.70	6/2460 (0.2%)
1	B	0.44	0/1831	0.76	8/2472 (0.3%)
1	C	0.45	0/1849	0.68	4/2496 (0.2%)
1	D	0.43	0/1828	0.69	4/2468 (0.2%)
All	All	0.44	0/7330	0.71	22/9896 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	LEU	CA-C-N	-9.43	106.99	122.65
1	B	95	LEU	C-N-CA	-9.43	106.99	122.65
1	A	197	ARG	CG-CD-NE	6.98	127.35	112.00
1	B	197	ARG	CG-CD-NE	6.98	127.35	112.00
1	D	197	ARG	CG-CD-NE	6.97	127.34	112.00
1	C	197	ARG	CG-CD-NE	6.96	127.32	112.00
1	C	198	LYS	CD-CE-NZ	5.62	129.88	111.90
1	B	198	LYS	CD-CE-NZ	5.62	129.87	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	198	LYS	CD-CE-NZ	5.61	129.84	111.90
1	A	198	LYS	CD-CE-NZ	5.59	129.79	111.90
1	A	187	GLU	CA-C-N	5.54	127.64	120.44
1	A	187	GLU	C-N-CA	5.54	127.64	120.44
1	A	15	ARG	CB-CG-CD	5.40	123.72	111.30
1	B	15	ARG	CB-CG-CD	5.40	123.72	111.30
1	C	15	ARG	CB-CG-CD	5.40	123.71	111.30
1	D	15	ARG	CB-CG-CD	5.39	123.69	111.30
1	B	187	GLU	CA-C-N	-5.33	111.62	120.68
1	B	187	GLU	C-N-CA	-5.33	111.62	120.68
1	B	15	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	C	15	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	15	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	D	15	ARG	NE-CZ-NH1	-5.20	116.30	121.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	SER	Peptide
1	B	193	SER	Peptide
1	C	193	SER	Peptide
1	D	193	SER	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	1800	0	1820	25	1
1	B	1806	0	1826	22	0
1	C	1824	0	1840	18	0
1	D	1803	0	1825	19	1
2	A	6	0	8	1	0
3	A	134	0	0	8	0
3	B	138	0	0	8	0
3	C	121	0	0	4	0
3	D	134	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7766	0	7319	75	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 5.

All (75) 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:244:ALA:OXT	3:B:301:HOH:O	1.84	0.95
1:D:64:ASP:OD2	3:D:301:HOH:O	2.02	0.77
1:C:102:ASP:OD1	3:C:301:HOH:O	2.05	0.73
1:D:102:ASP:OD1	3:D:302:HOH:O	2.05	0.73
1:B:151:TYR:OH	3:B:302:HOH:O	2.09	0.69
1:D:64:ASP:OD2	3:D:304:HOH:O	2.11	0.69
1:D:126:THR:O	3:D:303:HOH:O	2.10	0.68
1:B:225:ASP:O	3:B:303:HOH:O	2.12	0.67
1:D:145:ASN:OD1	1:D:148:GLN:OE1	2.13	0.66
1:A:183:PHE:HA	2:A:301:GOL:H12	1.78	0.66
1:D:14:SER:C	1:D:15:ARG:HG3	2.21	0.66
1:B:148:GLN:OE1	3:B:304:HOH:O	2.13	0.65
1:B:14:SER:C	1:B:15:ARG:HG3	2.21	0.65
1:A:173:GLN:OE1	3:A:401:HOH:O	2.15	0.65
1:A:14:SER:C	1:A:15:ARG:HG3	2.21	0.64
1:B:140:VAL:HG22	3:B:304:HOH:O	1.95	0.64
1:C:123:LYS:NZ	3:C:304:HOH:O	2.26	0.63
1:C:14:SER:C	1:C:15:ARG:HG3	2.21	0.62
1:C:145:ASN:HB2	1:C:146:PRO:HD2	1.81	0.61
1:A:225:ASP:O	3:A:402:HOH:O	2.16	0.59
1:C:47:ASP:OD2	3:C:302:HOH:O	2.17	0.59
1:B:127:LYS:HG2	3:B:427:HOH:O	2.04	0.57
1:A:93:ASN:HB2	3:A:406:HOH:O	2.05	0.57
1:A:144:ALA:HB2	1:B:163:ARG:HB3	1.86	0.57
1:A:5:ARG:NH1	1:A:52:GLN:HG2	2.21	0.56
1:A:202:ASP:OD1	3:A:403:HOH:O	2.18	0.56
1:B:93:ASN:HB2	3:B:310:HOH:O	2.07	0.54
1:D:126:THR:HG23	1:D:172:ARG:HD2	1.90	0.52
1:D:145:ASN:HB2	1:D:146:PRO:HD2	1.91	0.52
1:C:194:GLU:HA	1:C:197:ARG:NH1	2.25	0.51
1:D:194:GLU:HA	1:D:197:ARG:NH1	2.25	0.51
1:A:194:GLU:HA	1:A:197:ARG:NH1	2.25	0.51
1:A:146:PRO:CB	1:B:168[A]:GLU:HG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASN:CG	1:C:226:LYS:HD3	2.35	0.51
1:B:194:GLU:HA	1:B:197:ARG:NH1	2.25	0.50
1:A:142:HIS:ND1	3:A:409:HOH:O	2.34	0.50
1:A:173:GLN:O	3:A:404:HOH:O	2.19	0.50
1:C:144:ALA:HB2	1:D:163:ARG:HB3	1.93	0.49
1:A:146:PRO:HB3	1:B:168[A]:GLU:HG2	1.94	0.49
1:C:163:ARG:HB3	1:D:144:ALA:HB2	1.95	0.49
1:D:14:SER:C	1:D:15:ARG:CG	2.86	0.49
1:B:14:SER:C	1:B:15:ARG:CG	2.86	0.49
1:C:145:ASN:N	1:C:145:ASN:OD1	2.44	0.48
1:B:145:ASN:HB2	3:B:304:HOH:O	2.13	0.48
1:D:145:ASN:OD1	1:D:145:ASN:N	2.44	0.48
1:C:190:ASP:OD1	3:C:303:HOH:O	2.19	0.48
1:C:14:SER:C	1:C:15:ARG:CG	2.86	0.47
1:A:14:SER:C	1:A:15:ARG:CG	2.86	0.47
1:B:62:ASN:OD1	1:B:65:GLU:HG3	2.14	0.47
1:A:126:THR:HG23	1:A:172:ARG:HD2	1.98	0.45
1:A:5:ARG:HH12	1:A:52:GLN:HG2	1.83	0.44
1:A:119:LYS:HG3	1:B:96:LEU:HD23	2.00	0.44
1:A:144:ALA:HA	3:A:460:HOH:O	2.17	0.44
1:C:194:GLU:HA	1:C:197:ARG:HH12	1.83	0.44
1:A:194:GLU:HA	1:A:197:ARG:HH12	1.83	0.44
1:B:194:GLU:HA	1:B:197:ARG:HH12	1.83	0.44
1:D:128:ALA:O	1:D:129:ARG:HB2	2.18	0.44
1:B:89:ILE:HG21	1:B:109:ILE:HD13	2.01	0.43
1:C:188:MET:HE2	1:C:188:MET:HB3	1.76	0.43
1:C:94:LEU:HD22	1:D:168:GLU:HG2	1.99	0.43
1:D:194:GLU:HA	1:D:197:ARG:HH12	1.83	0.43
1:A:168:GLU:OE2	3:A:405:HOH:O	2.20	0.42
1:C:89:ILE:HG21	1:C:109:ILE:HD13	2.01	0.42
1:B:137:SER:HA	1:B:155:LYS:HD2	2.02	0.42
1:C:137:SER:HA	1:C:155:LYS:HD2	2.02	0.42
1:A:89:ILE:HG21	1:A:109:ILE:HD13	2.01	0.42
1:D:89:ILE:HG21	1:D:109:ILE:HD13	2.01	0.41
1:A:186:THR:OG1	1:A:188:MET:HB3	2.20	0.41
1:C:82:VAL:HG22	1:C:132:ARG:HB2	2.03	0.41
1:B:82:VAL:HG22	1:B:132:ARG:HB2	2.03	0.41
1:A:119:LYS:CG	1:B:96:LEU:HD23	2.51	0.41
1:D:82:VAL:HG22	1:D:132:ARG:HB2	2.03	0.41
1:A:137:SER:HA	1:A:155:LYS:HD2	2.02	0.40
1:D:137:SER:HA	1:D:155:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HG22	1:A:132:ARG:HB2	2.03	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:A:15:ARG:NH1	1:D:62:ASN:ND2[2_555]	1.80	0.40

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	238/244 (98%)	231 (97%)	6 (2%)	1 (0%)	30	19
1	B	239/244 (98%)	231 (97%)	7 (3%)	1 (0%)	30	19
1	C	241/244 (99%)	233 (97%)	7 (3%)	1 (0%)	30	19
1	D	239/244 (98%)	232 (97%)	6 (2%)	1 (0%)	30	19
All	All	957/976 (98%)	927 (97%)	26 (3%)	4 (0%)	30	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	B	194	GLU
1	C	194	GLU
1	D	194	GLU

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	188/192 (98%)	188 (100%)	0	100	100
1	B	189/192 (98%)	189 (100%)	0	100	100
1	C	191/192 (100%)	191 (100%)	0	100	100
1	D	189/192 (98%)	189 (100%)	0	100	100
All	All	757/768 (99%)	757 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	85	ASN
1	A	203	GLN
1	A	213	GLN
1	B	24	GLN
1	B	85	ASN
1	B	145	ASN
1	B	203	GLN
1	B	213	GLN
1	C	24	GLN
1	C	85	ASN
1	C	203	GLN
1	C	213	GLN
1	D	85	ASN
1	D	213	GLN

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

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	GOL	A	301	-	5,5,5	1.26	0	5,5,5	0.96	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	301	-	-	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
2	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GOL	1	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

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	240/244 (98%)	0.65	30 (12%) 8 6	16, 23, 58, 94	0
1	B	240/244 (98%)	0.65	31 (12%) 7 6	12, 23, 58, 94	1 (0%)
1	C	242/244 (99%)	0.65	32 (13%) 7 6	12, 23, 64, 94	1 (0%)
1	D	240/244 (98%)	0.60	27 (11%) 10 8	12, 23, 61, 94	1 (0%)
All	All	962/976 (98%)	0.64	120 (12%) 8 6	12, 23, 61, 94	3 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	191	ALA	8.7
1	B	96	LEU	7.1
1	B	192	LEU	6.3
1	A	15	ARG	5.8
1	D	62	ASN	5.8
1	A	191	ALA	5.2
1	D	196	ILE	5.0
1	B	193	SER	4.8
1	D	96	LEU	4.8
1	A	190	ASP	4.4
1	C	195	ASP	4.3
1	B	196	ILE	4.3
1	A	244	ALA	4.3
1	B	126	THR	4.2
1	C	196	ILE	4.1
1	A	143	PHE	4.1
1	B	195	ASP	4.1
1	C	189	THR	4.0
1	A	192	LEU	3.9
1	B	144	ALA	3.9
1	A	194	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	127	LYS	3.9
1	D	64	ASP	3.9
1	C	193	SER	3.9
1	C	51	GLU	3.8
1	B	62	ASN	3.8
1	A	198	LYS	3.7
1	A	144	ALA	3.7
1	C	244	ALA	3.7
1	B	194	GLU	3.7
1	A	197	ARG	3.6
1	D	143	PHE	3.6
1	C	191	ALA	3.6
1	C	192	LEU	3.5
1	B	244	ALA	3.5
1	C	190	ASP	3.5
1	C	127	LYS	3.4
1	D	144	ALA	3.4
1	A	187	GLU	3.4
1	A	51	GLU	3.4
1	D	187	GLU	3.4
1	A	193	SER	3.4
1	A	196	ILE	3.3
1	D	192	LEU	3.3
1	A	62	ASN	3.3
1	B	188	MET	3.3
1	B	143	PHE	3.3
1	D	193	SER	3.3
1	D	195	ASP	3.3
1	B	197	ARG	3.3
1	C	143	PHE	3.3
1	C	97	ARG	3.2
1	C	186	THR	3.2
1	C	188	MET	3.2
1	D	191	ALA	3.1
1	C	197	ARG	3.0
1	A	202	ASP	3.0
1	A	97	ARG	3.0
1	C	194	GLU	3.0
1	B	198	LYS	3.0
1	B	123	LYS	2.9
1	B	51	GLU	2.9
1	B	187	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	123	LYS	2.9
1	B	15	ARG	2.8
1	B	61	ARG	2.7
1	A	129	ARG	2.7
1	A	50	GLY	2.7
1	B	64	ASP	2.7
1	A	123	LYS	2.7
1	D	51	GLU	2.6
1	D	97	ARG	2.6
1	D	186	THR	2.6
1	A	61	ARG	2.6
1	B	128	ALA	2.6
1	A	64	ASP	2.5
1	C	142	HIS	2.5
1	B	60	VAL	2.5
1	C	3	GLN	2.5
1	A	142	HIS	2.5
1	A	188	MET	2.5
1	C	38	SER	2.5
1	C	145	ASN	2.5
1	A	195	ASP	2.5
1	D	190	ASP	2.5
1	A	186	THR	2.5
1	B	190	ASP	2.4
1	C	61	ARG	2.4
1	B	189	THR	2.4
1	C	187	GLU	2.4
1	C	198	LYS	2.4
1	C	144	ALA	2.4
1	B	225	ASP	2.4
1	D	188	MET	2.4
1	C	37	THR	2.3
1	D	197	ARG	2.3
1	D	244	ALA	2.3
1	A	148	GLN	2.3
1	D	128	ALA	2.3
1	D	194	GLU	2.3
1	D	142	HIS	2.2
1	B	142	HIS	2.2
1	A	52	GLN	2.2
1	D	61	ARG	2.2
1	A	201	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	45	LEU	2.2
1	C	77	TYR	2.2
1	D	189	THR	2.2
1	A	40	SER	2.2
1	C	52	GLN	2.1
1	C	5	ARG	2.1
1	B	170	GLY	2.1
1	B	186	THR	2.1
1	D	59	ASP	2.1
1	D	15	ARG	2.1
1	C	140	VAL	2.1
1	D	145	ASN	2.1
1	C	50	GLY	2.0
1	B	5	ARG	2.0
1	C	15	ARG	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	301	6/6	0.83	0.15	41,49,74,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.