



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:50 PM UTC

PDB ID : 3NO0 / pdb_00003no0
Title : Aquifex aeolicus type IIA topoisomerase C-terminal domain
Authors : Tretter, E.M.; Lerman, J.C.; Berger, J.M.
Deposited on : 2010-06-24
Resolution : 1.30 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

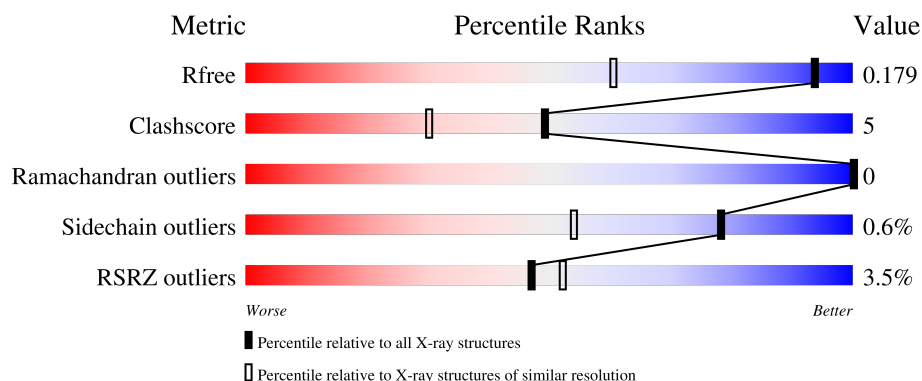
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	276	3% 91% 9%
1	B	276	3% 89% 9%
1	C	276	4% 87% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	7[B]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8021 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	22	0
			2292	1483	390	418	1			
1	B	276	Total	C	N	O	S	0	23	0
			2304	1493	391	419	1			
1	C	276	Total	C	N	O	S	0	40	0
			2401	1566	403	430	2			

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	733	ASP	-	SEE REMARK 999	UNP O67108
A	734	LYS	-	SEE REMARK 999	UNP O67108
A	735	ILE	-	SEE REMARK 999	UNP O67108
A	736	ASN	-	SEE REMARK 999	UNP O67108
A	737	GLN	-	SEE REMARK 999	UNP O67108
A	738	LYS	-	SEE REMARK 999	UNP O67108
A	739	ASP	-	SEE REMARK 999	UNP O67108
A	740	ILE	-	SEE REMARK 999	UNP O67108
A	741	PRO	-	SEE REMARK 999	UNP O67108
A	742	LEU	-	SEE REMARK 999	UNP O67108
A	743	SER	-	SEE REMARK 999	UNP O67108
A	744	THR	-	SEE REMARK 999	UNP O67108
A	745	LYS	-	SEE REMARK 999	UNP O67108
A	746	LYS	-	SEE REMARK 999	UNP O67108
A	747	SER	-	SEE REMARK 999	UNP O67108
A	748	ILE	-	SEE REMARK 999	UNP O67108
A	749	PRO	-	SEE REMARK 999	UNP O67108
A	750	ARG	-	SEE REMARK 999	UNP O67108
A	751	THR	-	SEE REMARK 999	UNP O67108
A	752	ARG	-	SEE REMARK 999	UNP O67108
A	753	TRP	-	SEE REMARK 999	UNP O67108
A	754	LYS	-	SEE REMARK 999	UNP O67108
A	755	LEU	-	SEE REMARK 999	UNP O67108

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Chain	Residue	Modelled	Actual	Comment	Reference
A	756	GLU	-	SEE REMARK 999	UNP O67108
A	757	ASP	-	SEE REMARK 999	UNP O67108
A	758	ASP	-	SEE REMARK 999	UNP O67108
A	759	GLU	-	SEE REMARK 999	UNP O67108
A	760	ILE	-	SEE REMARK 999	UNP O67108
A	761	ILE	-	SEE REMARK 999	UNP O67108
A	762	LYS	-	SEE REMARK 999	UNP O67108
A	763	VAL	-	SEE REMARK 999	UNP O67108
A	764	VAL	-	SEE REMARK 999	UNP O67108
A	765	ILE	-	SEE REMARK 999	UNP O67108
A	766	LYS	-	SEE REMARK 999	UNP O67108
A	767	LYS	-	SEE REMARK 999	UNP O67108
A	768	SER	-	SEE REMARK 999	UNP O67108
A	769	GLU	-	SEE REMARK 999	UNP O67108
B	733	ASP	-	SEE REMARK 999	UNP O67108
B	734	LYS	-	SEE REMARK 999	UNP O67108
B	735	ILE	-	SEE REMARK 999	UNP O67108
B	736	ASN	-	SEE REMARK 999	UNP O67108
B	737	GLN	-	SEE REMARK 999	UNP O67108
B	738	LYS	-	SEE REMARK 999	UNP O67108
B	739	ASP	-	SEE REMARK 999	UNP O67108
B	740	ILE	-	SEE REMARK 999	UNP O67108
B	741	PRO	-	SEE REMARK 999	UNP O67108
B	742	LEU	-	SEE REMARK 999	UNP O67108
B	743	SER	-	SEE REMARK 999	UNP O67108
B	744	THR	-	SEE REMARK 999	UNP O67108
B	745	LYS	-	SEE REMARK 999	UNP O67108
B	746	LYS	-	SEE REMARK 999	UNP O67108
B	747	SER	-	SEE REMARK 999	UNP O67108
B	748	ILE	-	SEE REMARK 999	UNP O67108
B	749	PRO	-	SEE REMARK 999	UNP O67108
B	750	ARG	-	SEE REMARK 999	UNP O67108
B	751	THR	-	SEE REMARK 999	UNP O67108
B	752	ARG	-	SEE REMARK 999	UNP O67108
B	753	TRP	-	SEE REMARK 999	UNP O67108
B	754	LYS	-	SEE REMARK 999	UNP O67108
B	755	LEU	-	SEE REMARK 999	UNP O67108
B	756	GLU	-	SEE REMARK 999	UNP O67108
B	757	ASP	-	SEE REMARK 999	UNP O67108
B	758	ASP	-	SEE REMARK 999	UNP O67108
B	759	GLU	-	SEE REMARK 999	UNP O67108
B	760	ILE	-	SEE REMARK 999	UNP O67108

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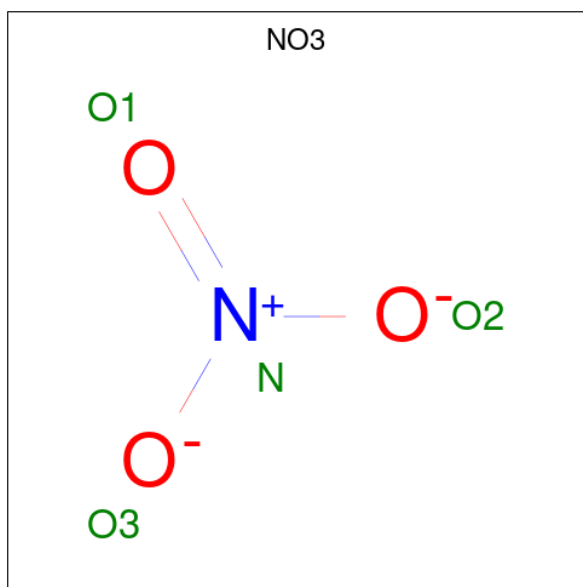
Chain	Residue	Modelled	Actual	Comment	Reference
B	761	ILE	-	SEE REMARK 999	UNP O67108
B	762	LYS	-	SEE REMARK 999	UNP O67108
B	763	VAL	-	SEE REMARK 999	UNP O67108
B	764	VAL	-	SEE REMARK 999	UNP O67108
B	765	ILE	-	SEE REMARK 999	UNP O67108
B	766	LYS	-	SEE REMARK 999	UNP O67108
B	767	LYS	-	SEE REMARK 999	UNP O67108
B	768	SER	-	SEE REMARK 999	UNP O67108
B	769	GLU	-	SEE REMARK 999	UNP O67108
C	733	ASP	-	SEE REMARK 999	UNP O67108
C	734	LYS	-	SEE REMARK 999	UNP O67108
C	735	ILE	-	SEE REMARK 999	UNP O67108
C	736	ASN	-	SEE REMARK 999	UNP O67108
C	737	GLN	-	SEE REMARK 999	UNP O67108
C	738	LYS	-	SEE REMARK 999	UNP O67108
C	739	ASP	-	SEE REMARK 999	UNP O67108
C	740	ILE	-	SEE REMARK 999	UNP O67108
C	741	PRO	-	SEE REMARK 999	UNP O67108
C	742	LEU	-	SEE REMARK 999	UNP O67108
C	743	SER	-	SEE REMARK 999	UNP O67108
C	744	THR	-	SEE REMARK 999	UNP O67108
C	745	LYS	-	SEE REMARK 999	UNP O67108
C	746	LYS	-	SEE REMARK 999	UNP O67108
C	747	SER	-	SEE REMARK 999	UNP O67108
C	748	ILE	-	SEE REMARK 999	UNP O67108
C	749	PRO	-	SEE REMARK 999	UNP O67108
C	750	ARG	-	SEE REMARK 999	UNP O67108
C	751	THR	-	SEE REMARK 999	UNP O67108
C	752	ARG	-	SEE REMARK 999	UNP O67108
C	753	TRP	-	SEE REMARK 999	UNP O67108
C	754	LYS	-	SEE REMARK 999	UNP O67108
C	755	LEU	-	SEE REMARK 999	UNP O67108
C	756	GLU	-	SEE REMARK 999	UNP O67108
C	757	ASP	-	SEE REMARK 999	UNP O67108
C	758	ASP	-	SEE REMARK 999	UNP O67108
C	759	GLU	-	SEE REMARK 999	UNP O67108
C	760	ILE	-	SEE REMARK 999	UNP O67108
C	761	ILE	-	SEE REMARK 999	UNP O67108
C	762	LYS	-	SEE REMARK 999	UNP O67108
C	763	VAL	-	SEE REMARK 999	UNP O67108
C	764	VAL	-	SEE REMARK 999	UNP O67108
C	765	ILE	-	SEE REMARK 999	UNP O67108

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Chain	Residue	Modelled	Actual	Comment	Reference
C	766	LYS	-	SEE REMARK 999	UNP O67108
C	767	LYS	-	SEE REMARK 999	UNP O67108
C	768	SER	-	SEE REMARK 999	UNP O67108
C	769	GLU	-	SEE REMARK 999	UNP O67108

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	B	1	Total	N	O	0	0
			4	1	3		
2	C	1	Total	N	O	0	0
			4	1	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	1
			12	6	6		
3	C	1	Total	C	O	0	0
			6	3	3		

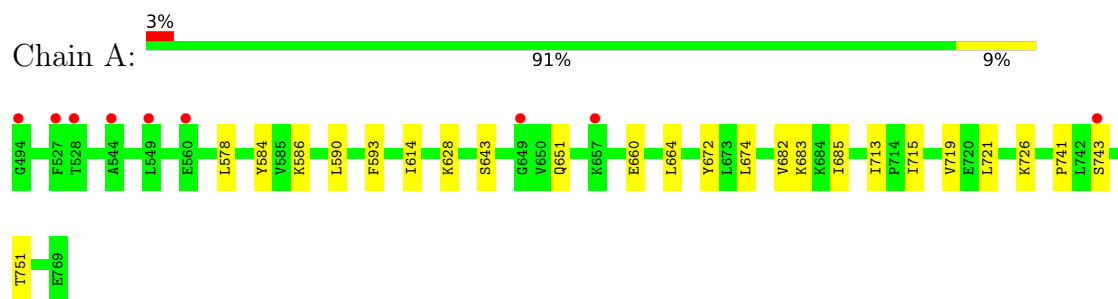
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	316	Total	O	0	0
			316	316		
4	B	279	Total	O	0	0
			279	279		
4	C	353	Total	O	0	0
			353	353		

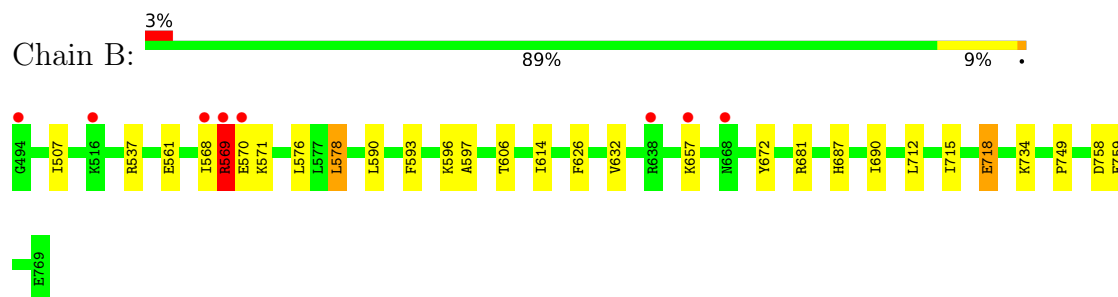
3 Residue-property plots [i](#)

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.

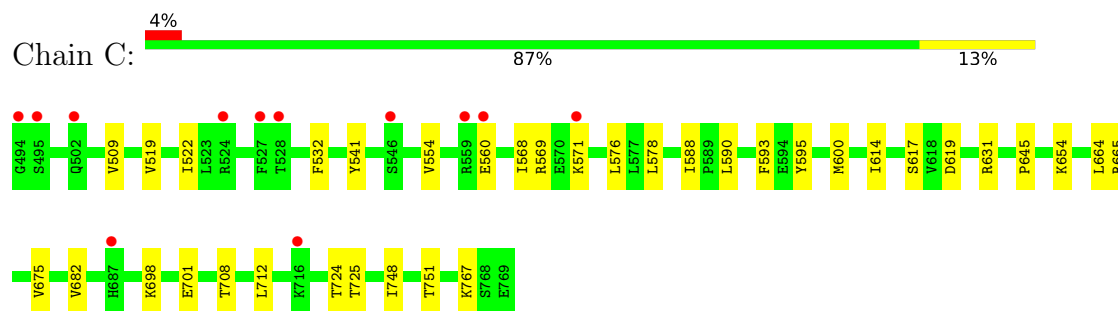
- Molecule 1: DNA gyrase subunit A



- Molecule 1: DNA gyrase subunit A



- Molecule 1: DNA gyrase subunit A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.51Å 49.62Å 120.35Å 91.57° 99.75° 113.48°	Depositor
Resolution (Å)	40.85 – 1.30 40.85 – 1.30	Depositor EDS
% Data completeness (in resolution range)	93.5 (40.85-1.30) 93.5 (40.85-1.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.172 , 0.189 0.163 , 0.179	Depositor DCC
R_{free} test set	10451 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8021	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 5.79% 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, NO3

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	0.70	2/2375 (0.1%)	0.77	3/3198 (0.1%)
1	B	0.79	6/2393 (0.3%)	0.82	5/3223 (0.2%)
1	C	0.80	0/2531	0.79	0/3407
All	All	0.77	8/7299 (0.1%)	0.79	8/9828 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	LEU	C-O	-7.22	1.15	1.24
1	B	687	HIS	C-O	-6.30	1.16	1.24
1	B	718	GLU	C-O	-5.86	1.16	1.23
1	A	741	PRO	C-N	-5.33	1.25	1.33
1	B	578[A]	LEU	C-O	-5.19	1.17	1.23
1	B	578[B]	LEU	C-O	-5.19	1.17	1.23
1	B	569	ARG	C-N	-5.13	1.27	1.33
1	B	596	LYS	C-O	-5.11	1.16	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	569	ARG	CA-C-O	7.38	128.37	120.55
1	A	593	PHE	N-CA-CB	-6.09	102.95	110.98
1	B	570	GLU	N-CA-C	5.98	117.80	111.28
1	B	568	ILE	O-C-N	-5.52	117.51	123.14
1	B	597	ALA	CA-C-N	5.28	128.21	120.71
1	B	597	ALA	C-N-CA	5.28	128.21	120.71
1	A	593	PHE	N-CA-C	5.19	121.91	114.39
1	A	713	ILE	N-CA-C	5.07	112.88	107.76

There are no chirality outliers.

There are no planarity outliers.

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	2292	0	2491	16	0
1	B	2304	0	2518	20	0
1	C	2401	0	2677	44	0
2	A	4	0	0	0	0
2	B	8	0	0	0	0
2	C	4	0	0	0	0
3	A	12	0	16	0	0
3	B	12	0	16	1	0
3	C	36	0	43	6	0
4	A	316	0	0	3	0
4	B	279	0	0	0	0
4	C	353	0	0	8	0
All	All	8021	0	7761	80	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 5.

All (80) 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:C:708[B]:THR:HG22	4:C:955:HOH:O	1.59	1.03
1:B:569:ARG:HD2	1:B:590[B]:LEU:HD13	1.42	1.00
1:B:569:ARG:HD2	1:B:590[A]:LEU:HD23	1.43	0.99
1:A:584[B]:TYR:CZ	1:A:651:GLN:NE2	2.46	0.84
1:C:519:VAL:O	1:C:724[B]:THR:HG21	1.87	0.75
1:C:569[B]:ARG:NH1	4:C:811:HOH:O	2.24	0.71
1:C:568[A]:ILE:HG13	1:C:571[A]:LYS:HB2	1.75	0.68
1:C:588[B]:ILE:HD11	1:C:645:PRO:HG3	1.80	0.63
1:C:578[A]:LEU:CD2	1:C:614:ILE:HG22	2.29	0.62
1:C:654[B]:LYS:HG3	1:C:698:LYS:HZ3	1.64	0.62
1:A:578[B]:LEU:HD23	1:A:614:ILE:HG22	1.81	0.61
1:C:571[B]:LYS:O	1:C:571[B]:LYS:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578[A]:LEU:HD23	1:C:614:ILE:HG22	1.83	0.59
1:C:568[A]:ILE:HD11	1:C:571[A]:LYS:HD3	1.86	0.58
1:C:519:VAL:HB	1:C:724[B]:THR:HG21	1.86	0.56
1:C:619:ASP:HA	3:C:7[B]:GOL:H32	1.87	0.56
1:B:576[B]:LEU:HD11	1:B:614:ILE:HB	1.86	0.56
1:C:532:PHE:CE2	1:C:569[B]:ARG:HB2	2.41	0.56
1:B:632[B]:VAL:HG21	1:B:690:ILE:HD13	1.86	0.56
1:C:619:ASP:CA	3:C:7[B]:GOL:H32	2.36	0.55
1:B:626:PHE:HB3	1:B:632[B]:VAL:HG12	1.89	0.54
1:C:519:VAL:HB	1:C:724[B]:THR:CG2	2.38	0.54
1:A:578[B]:LEU:CD2	1:A:614:ILE:HG22	2.39	0.53
1:C:724[B]:THR:CG2	4:C:963:HOH:O	2.56	0.52
1:C:617:SER:CB	3:C:7[B]:GOL:H2	2.40	0.52
1:B:569:ARG:HH11	1:B:590[B]:LEU:HD13	1.74	0.52
1:C:541:TYR:CG	1:C:554[B]:VAL:HG11	2.44	0.51
1:C:617:SER:HB3	3:C:7[B]:GOL:H2	1.92	0.51
1:A:672:TYR:HB2	1:A:715:ILE:HG23	1.92	0.51
1:C:569[A]:ARG:HD3	1:C:595:TYR:CE2	2.46	0.50
1:B:632[B]:VAL:CG1	1:B:712[B]:LEU:HD11	2.41	0.50
1:C:665:ARG:HG3	1:C:712:LEU:O	2.11	0.49
1:C:560[C]:GLU:CD	1:C:560[C]:GLU:O	2.55	0.49
1:C:631[A]:ARG:HG3	1:C:701:GLU:HG2	1.95	0.49
1:A:751[B]:THR:HG22	4:A:455:HOH:O	2.13	0.48
1:B:590[B]:LEU:HD23	1:B:593:PHE:CZ	2.48	0.48
1:C:751[B]:THR:HG22	4:C:280:HOH:O	2.13	0.48
1:B:626:PHE:CD2	1:B:712[B]:LEU:HD12	2.49	0.48
1:C:576[A]:LEU:HD11	1:C:614:ILE:HB	1.95	0.48
1:B:569:ARG:HH11	1:B:590[B]:LEU:CD1	2.26	0.47
1:C:568[A]:ILE:CD1	1:C:571[A]:LYS:HD3	2.44	0.47
1:C:541:TYR:CB	1:C:554[B]:VAL:HG11	2.45	0.47
1:C:571[B]:LYS:HG2	4:C:784:HOH:O	2.15	0.47
1:B:758:ASP:C	1:B:759[A]:GLU:HG3	2.41	0.46
1:C:569[A]:ARG:CD	1:C:595:TYR:CE2	2.99	0.45
1:C:532:PHE:CE2	1:C:569[A]:ARG:HB2	2.51	0.45
1:C:724[B]:THR:HG22	1:C:725:THR:N	2.31	0.45
1:B:606:THR:HG23	3:B:9:GOL:H2	1.98	0.45
1:C:590[B]:LEU:HD13	1:C:593:PHE:CZ	2.52	0.45
1:A:674[B]:LEU:HD11	1:A:682[B]:VAL:HB	1.99	0.44
1:A:674[B]:LEU:HD12	1:A:683:LYS:O	2.17	0.44
1:C:748:ILE:HD13	3:C:6:GOL:H11	1.99	0.44
1:C:569[B]:ARG:NH2	1:C:569[B]:ARG:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:ASP:N	3:C:7[B]:GOL:H32	2.33	0.43
1:B:758:ASP:O	1:B:759[A]:GLU:HG3	2.17	0.43
1:C:569[A]:ARG:HD3	1:C:595:TYR:HE2	1.81	0.43
1:A:628[A]:LYS:HD3	1:A:660:GLU:HG2	2.00	0.43
1:B:718:GLU:OE2	1:B:734[A]:LYS:HD3	2.18	0.43
1:B:537[B]:ARG:HG3	1:B:561:GLU:CG	2.48	0.43
1:A:664:LEU:C	1:A:664:LEU:HD23	2.44	0.43
1:A:719[B]:VAL:HG11	1:A:721:LEU:HD21	2.01	0.43
1:C:708[A]:THR:HG21	4:C:864:HOH:O	2.19	0.42
1:C:541:TYR:CD1	1:C:554[B]:VAL:CG1	3.03	0.42
1:B:632[B]:VAL:HG11	1:B:712[B]:LEU:HD11	2.01	0.41
1:C:509[B]:VAL:CG2	1:C:522:ILE:HG23	2.50	0.41
1:A:586:LYS:HE3	1:A:643:SER:OG	2.20	0.41
1:B:672:TYR:HB2	1:B:715:ILE:HG23	2.02	0.41
1:A:685:ILE:HG22	1:A:743:SER:O	2.21	0.41
1:A:751[C]:THR:HG22	4:A:813:HOH:O	2.19	0.41
1:A:726:LYS:HG3	4:A:267:HOH:O	2.20	0.41
1:C:600[B]:MET:HE1	4:C:851:HOH:O	2.20	0.41
1:B:681:ARG:HB3	1:B:749:PRO:HB2	2.02	0.40
1:A:584[B]:TYR:OH	1:A:651:GLN:NE2	2.54	0.40
1:C:767[B]:LYS:NZ	4:C:815:HOH:O	2.54	0.40
1:C:675:VAL:O	1:C:682:VAL:HA	2.21	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	296/276 (107%)	292 (99%)	4 (1%)	0	100	100
1	B	298/276 (108%)	292 (98%)	6 (2%)	0	100	100
1	C	315/276 (114%)	309 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	909/828 (110%)	893 (98%)	16 (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	262/241 (109%)	262 (100%)	0	100	100
1	B	265/241 (110%)	260 (98%)	5 (2%)	50	14
1	C	282/241 (117%)	282 (100%)	0	100	100
All	All	809/723 (112%)	804 (99%)	5 (1%)	78	54

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	507[A]	ILE
1	B	507[B]	ILE
1	B	569	ARG
1	B	571	LYS
1	B	657	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	550	GLN
1	A	651	GLN
1	A	658	ASN
1	B	547	GLN
1	C	694	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 ⓘ

14 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
3	GOL	B	770	-	5,5,5	0.33	0	5,5,5	0.45	0
2	NO3	B	2	-	1,3,3	2.60	1 (100%)	0,3,3	-	-
3	GOL	C	7[B]	-	5,5,5	0.62	0	5,5,5	1.37	1 (20%)
2	NO3	B	4	-	1,3,3	3.10	1 (100%)	0,3,3	-	-
3	GOL	C	5	-	5,5,5	0.47	0	5,5,5	0.37	0
3	GOL	A	4	-	5,5,5	0.34	0	5,5,5	0.35	0
3	GOL	C	8	-	5,5,5	1.37	1 (20%)	5,5,5	0.57	0
3	GOL	A	1	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	C	6	-	5,5,5	1.81	1 (20%)	5,5,5	2.85	1 (20%)
3	GOL	C	3	-	5,5,5	0.71	0	5,5,5	0.54	0
3	GOL	C	7[A]	-	5,5,5	0.37	0	5,5,5	0.60	0
3	GOL	B	9	-	5,5,5	0.86	0	5,5,5	1.39	1 (20%)
2	NO3	A	3	-	1,3,3	2.92	1 (100%)	0,3,3	-	-
2	NO3	C	1	-	1,3,3	3.01	1 (100%)	0,3,3	-	-

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	B	770	-	-	0/4/4/4	-
3	GOL	C	7[B]	-	-	2/4/4/4	-
3	GOL	C	5	-	-	0/4/4/4	-
3	GOL	A	4	-	-	0/4/4/4	-
3	GOL	C	8	-	-	2/4/4/4	-
3	GOL	A	1	-	-	0/4/4/4	-
3	GOL	C	6	-	-	2/4/4/4	-
3	GOL	C	3	-	-	0/4/4/4	-
3	GOL	C	7[A]	-	-	0/4/4/4	-
3	GOL	B	9	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	NO3	O1-N	3.10	1.39	1.24
3	C	6	GOL	O2-C2	-3.05	1.34	1.43
2	C	1	NO3	O1-N	3.01	1.39	1.24
2	A	3	NO3	O1-N	2.92	1.38	1.24
2	B	2	NO3	O1-N	2.60	1.37	1.24
3	C	8	GOL	O2-C2	-2.56	1.35	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	GOL	O2-C2-C3	6.08	134.33	109.18
3	B	9	GOL	O2-C2-C1	2.60	119.95	109.18
3	C	7[B]	GOL	O2-C2-C3	-2.45	99.02	109.18

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	9	GOL	C1-C2-C3-O3
3	C	6	GOL	O2-C2-C3-O3
3	C	7[B]	GOL	O1-C1-C2-C3
3	C	8	GOL	C1-C2-C3-O3
3	C	8	GOL	O2-C2-C3-O3
3	C	7[B]	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	9	GOL	O1-C1-C2-O2
3	C	6	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	7[B]	GOL	5	0
3	C	6	GOL	1	0
3	B	9	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	276/276 (100%)	0.19	9 (3%)	49	55	7, 18, 40, 65	23 (8%)
1	B	276/276 (100%)	0.19	8 (2%)	53	60	7, 19, 39, 62	24 (8%)
1	C	276/276 (100%)	-0.05	12 (4%)	40	45	4, 13, 28, 53	45 (16%)
All	All	828/828 (100%)	0.11	29 (3%)	47	52	4, 17, 36, 65	92 (11%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	527	PHE	5.6
1	C	571[A]	LYS	4.4
1	B	568	ILE	4.3
1	A	743	SER	4.2
1	C	494	GLY	4.0
1	C	687	HIS	3.9
1	C	560[A]	GLU	3.7
1	A	494	GLY	3.4
1	C	527	PHE	3.2
1	B	569	ARG	3.1
1	C	546	SER	3.0
1	B	516	LYS	2.9
1	A	528	THR	2.9
1	B	570	GLU	2.6
1	C	495	SER	2.5
1	A	649[A]	GLY	2.4
1	B	494	GLY	2.4
1	C	716	LYS	2.3
1	A	544	ALA	2.2
1	B	657	LYS	2.2
1	B	668	ASN	2.2
1	A	560	GLU	2.1
1	A	549	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	528	THR	2.1
1	C	502	GLN	2.1
1	A	657	LYS	2.1
1	B	638	ARG	2.0
1	C	524	ARG	2.0
1	C	559	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(Å ²)	Q<0.9
3	GOL	C	6	6/6	0.74	0.22	21,27,40,40	0
3	GOL	C	5	6/6	0.83	0.15	24,27,28,28	6
3	GOL	A	4	6/6	0.87	0.16	24,26,28,29	6
3	GOL	C	8	6/6	0.87	0.17	12,33,40,40	0
2	NO3	B	2	4/4	0.89	0.12	19,19,19,21	4
2	NO3	B	4	4/4	0.89	0.10	28,30,34,36	0
3	GOL	B	770	6/6	0.90	0.13	16,18,22,24	6
3	GOL	B	9	6/6	0.90	0.12	25,36,41,46	0
3	GOL	C	3	6/6	0.90	0.10	10,14,18,20	6
3	GOL	A	1	6/6	0.91	0.10	13,17,18,19	6
3	GOL	C	7[A]	6/6	0.94	0.10	10,14,18,20	6
3	GOL	C	7[B]	6/6	0.94	0.10	18,25,33,35	6
2	NO3	A	3	4/4	0.94	0.12	24,24,25,28	4
2	NO3	C	1	4/4	0.96	0.07	19,21,22,22	4

6.5 Other polymers [i](#)

There are no such residues in this entry.