



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:51 pm BST

PDB ID : 2WSU
Title : Galectin domain of porcine adenovirus type 4 NADC-1 isolate fibre
Authors : Guardado-Calvo, P.; Munoz, E.M.; Llamas-Saiz, A.L.; Fox, G.C.; Glasgow, J.N.; van Raaij, M.J.
Deposited on : 2009-09-10
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

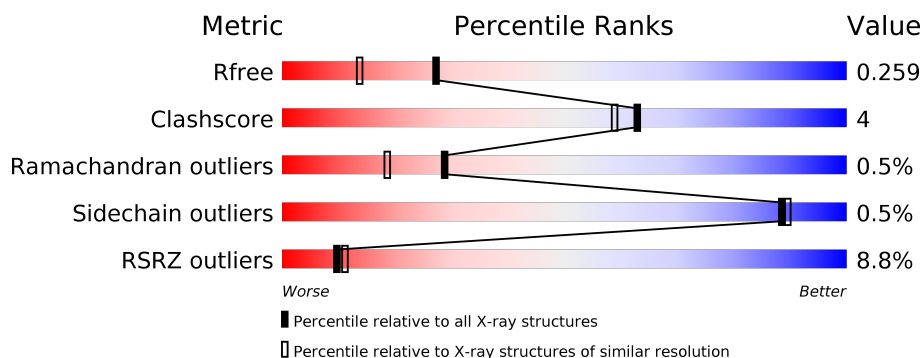
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	343	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>13%</div> </div> </div>
1	B	343	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>11%</div> </div> </div>
1	C	343	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>6%</div> <div>11%</div> </div> </div>
1	D	343	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10265 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 PUTATIVE FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	1	0
			2366	1530	398	433	5			
1	B	306	Total	C	N	O	S	0	1	0
			2408	1557	404	442	5			
1	C	306	Total	C	N	O	S	0	2	0
			2420	1564	405	446	5			
1	D	299	Total	C	N	O	S	0	2	0
			2362	1526	398	433	5			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	MET	-	expression tag	UNP Q83467
A	362	GLY	-	expression tag	UNP Q83467
A	363	SER	-	expression tag	UNP Q83467
A	364	SER	-	expression tag	UNP Q83467
A	365	HIS	-	expression tag	UNP Q83467
A	366	HIS	-	expression tag	UNP Q83467
A	367	HIS	-	expression tag	UNP Q83467
A	368	HIS	-	expression tag	UNP Q83467
A	369	HIS	-	expression tag	UNP Q83467
A	370	HIS	-	expression tag	UNP Q83467
A	371	SER	-	expression tag	UNP Q83467
A	372	SER	-	expression tag	UNP Q83467
A	373	GLY	-	expression tag	UNP Q83467
A	374	LEU	-	expression tag	UNP Q83467
A	375	VAL	-	expression tag	UNP Q83467
A	376	PRO	-	expression tag	UNP Q83467
A	377	ARG	-	expression tag	UNP Q83467
A	378	GLY	-	expression tag	UNP Q83467
A	379	SER	-	expression tag	UNP Q83467
A	380	HIS	-	expression tag	UNP Q83467
A	381	MET	-	expression tag	UNP Q83467

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Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ALA	-	expression tag	UNP Q83467
A	383	SER	-	expression tag	UNP Q83467
A	384	MET	-	expression tag	UNP Q83467
A	385	THR	-	expression tag	UNP Q83467
A	386	GLY	-	expression tag	UNP Q83467
A	387	GLY	-	expression tag	UNP Q83467
A	388	GLN	-	expression tag	UNP Q83467
A	389	GLN	-	expression tag	UNP Q83467
A	390	GLY	-	expression tag	UNP Q83467
A	391	ARG	-	expression tag	UNP Q83467
A	392	ILE	-	expression tag	UNP Q83467
B	361	MET	-	expression tag	UNP Q83467
B	362	GLY	-	expression tag	UNP Q83467
B	363	SER	-	expression tag	UNP Q83467
B	364	SER	-	expression tag	UNP Q83467
B	365	HIS	-	expression tag	UNP Q83467
B	366	HIS	-	expression tag	UNP Q83467
B	367	HIS	-	expression tag	UNP Q83467
B	368	HIS	-	expression tag	UNP Q83467
B	369	HIS	-	expression tag	UNP Q83467
B	370	HIS	-	expression tag	UNP Q83467
B	371	SER	-	expression tag	UNP Q83467
B	372	SER	-	expression tag	UNP Q83467
B	373	GLY	-	expression tag	UNP Q83467
B	374	LEU	-	expression tag	UNP Q83467
B	375	VAL	-	expression tag	UNP Q83467
B	376	PRO	-	expression tag	UNP Q83467
B	377	ARG	-	expression tag	UNP Q83467
B	378	GLY	-	expression tag	UNP Q83467
B	379	SER	-	expression tag	UNP Q83467
B	380	HIS	-	expression tag	UNP Q83467
B	381	MET	-	expression tag	UNP Q83467
B	382	ALA	-	expression tag	UNP Q83467
B	383	SER	-	expression tag	UNP Q83467
B	384	MET	-	expression tag	UNP Q83467
B	385	THR	-	expression tag	UNP Q83467
B	386	GLY	-	expression tag	UNP Q83467
B	387	GLY	-	expression tag	UNP Q83467
B	388	GLN	-	expression tag	UNP Q83467
B	389	GLN	-	expression tag	UNP Q83467
B	390	GLY	-	expression tag	UNP Q83467
B	391	ARG	-	expression tag	UNP Q83467

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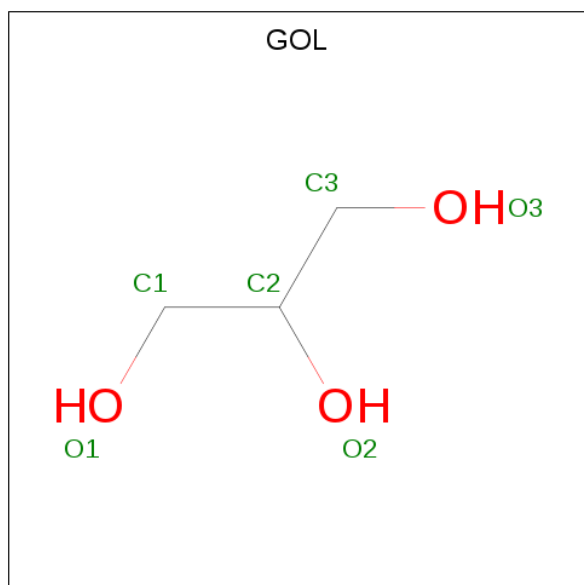
Chain	Residue	Modelled	Actual	Comment	Reference
B	392	ILE	-	expression tag	UNP Q83467
C	361	MET	-	expression tag	UNP Q83467
C	362	GLY	-	expression tag	UNP Q83467
C	363	SER	-	expression tag	UNP Q83467
C	364	SER	-	expression tag	UNP Q83467
C	365	HIS	-	expression tag	UNP Q83467
C	366	HIS	-	expression tag	UNP Q83467
C	367	HIS	-	expression tag	UNP Q83467
C	368	HIS	-	expression tag	UNP Q83467
C	369	HIS	-	expression tag	UNP Q83467
C	370	HIS	-	expression tag	UNP Q83467
C	371	SER	-	expression tag	UNP Q83467
C	372	SER	-	expression tag	UNP Q83467
C	373	GLY	-	expression tag	UNP Q83467
C	374	LEU	-	expression tag	UNP Q83467
C	375	VAL	-	expression tag	UNP Q83467
C	376	PRO	-	expression tag	UNP Q83467
C	377	ARG	-	expression tag	UNP Q83467
C	378	GLY	-	expression tag	UNP Q83467
C	379	SER	-	expression tag	UNP Q83467
C	380	HIS	-	expression tag	UNP Q83467
C	381	MET	-	expression tag	UNP Q83467
C	382	ALA	-	expression tag	UNP Q83467
C	383	SER	-	expression tag	UNP Q83467
C	384	MET	-	expression tag	UNP Q83467
C	385	THR	-	expression tag	UNP Q83467
C	386	GLY	-	expression tag	UNP Q83467
C	387	GLY	-	expression tag	UNP Q83467
C	388	GLN	-	expression tag	UNP Q83467
C	389	GLN	-	expression tag	UNP Q83467
C	390	GLY	-	expression tag	UNP Q83467
C	391	ARG	-	expression tag	UNP Q83467
C	392	ILE	-	expression tag	UNP Q83467
D	361	MET	-	expression tag	UNP Q83467
D	362	GLY	-	expression tag	UNP Q83467
D	363	SER	-	expression tag	UNP Q83467
D	364	SER	-	expression tag	UNP Q83467
D	365	HIS	-	expression tag	UNP Q83467
D	366	HIS	-	expression tag	UNP Q83467
D	367	HIS	-	expression tag	UNP Q83467
D	368	HIS	-	expression tag	UNP Q83467
D	369	HIS	-	expression tag	UNP Q83467

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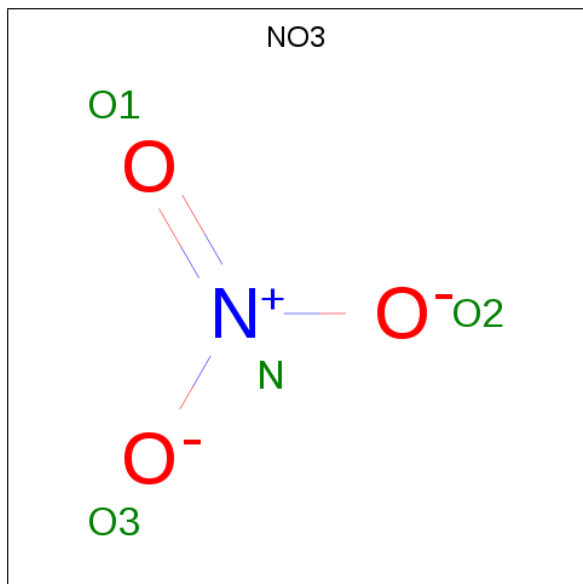
Chain	Residue	Modelled	Actual	Comment	Reference
D	370	HIS	-	expression tag	UNP Q83467
D	371	SER	-	expression tag	UNP Q83467
D	372	SER	-	expression tag	UNP Q83467
D	373	GLY	-	expression tag	UNP Q83467
D	374	LEU	-	expression tag	UNP Q83467
D	375	VAL	-	expression tag	UNP Q83467
D	376	PRO	-	expression tag	UNP Q83467
D	377	ARG	-	expression tag	UNP Q83467
D	378	GLY	-	expression tag	UNP Q83467
D	379	SER	-	expression tag	UNP Q83467
D	380	HIS	-	expression tag	UNP Q83467
D	381	MET	-	expression tag	UNP Q83467
D	382	ALA	-	expression tag	UNP Q83467
D	383	SER	-	expression tag	UNP Q83467
D	384	MET	-	expression tag	UNP Q83467
D	385	THR	-	expression tag	UNP Q83467
D	386	GLY	-	expression tag	UNP Q83467
D	387	GLY	-	expression tag	UNP Q83467
D	388	GLN	-	expression tag	UNP Q83467
D	389	GLN	-	expression tag	UNP Q83467
D	390	GLY	-	expression tag	UNP Q83467
D	391	ARG	-	expression tag	UNP Q83467
D	392	ILE	-	expression tag	UNP Q83467

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		

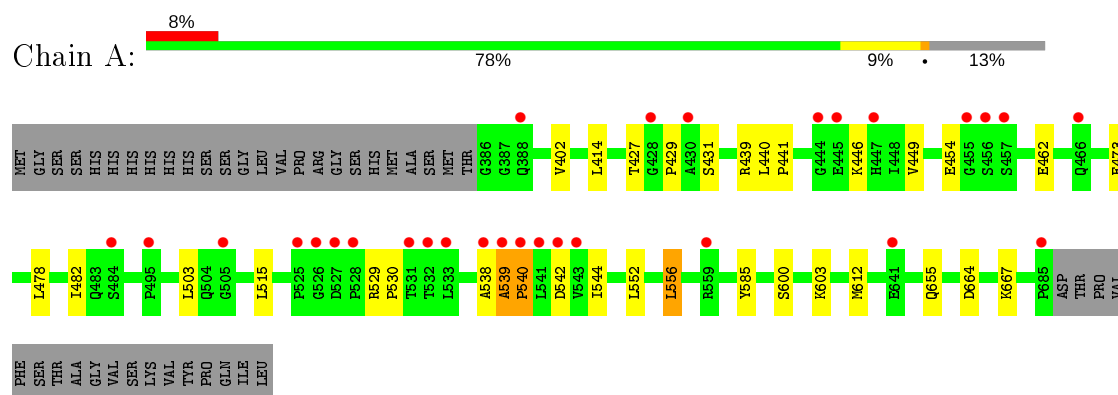
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	168	Total	O	0	0
			168	168		
4	C	160	Total	O	0	0
			160	160		
4	D	142	Total	O	0	0
			142	142		

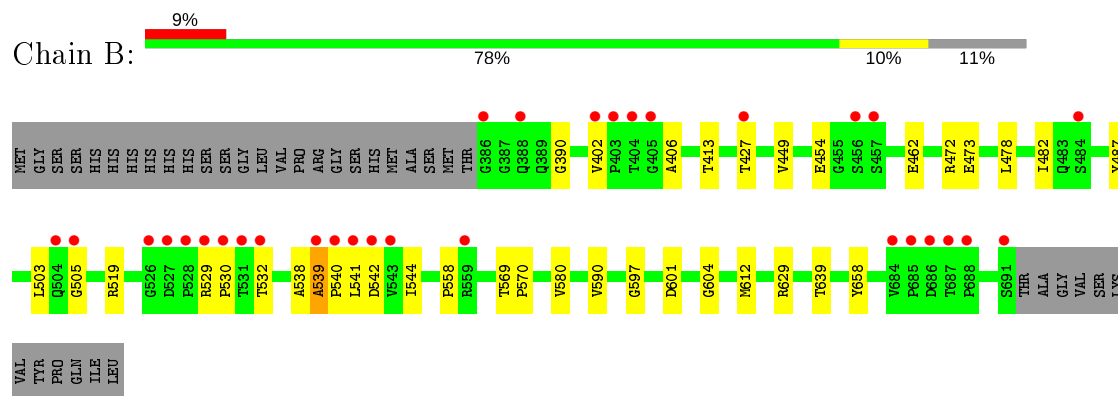
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

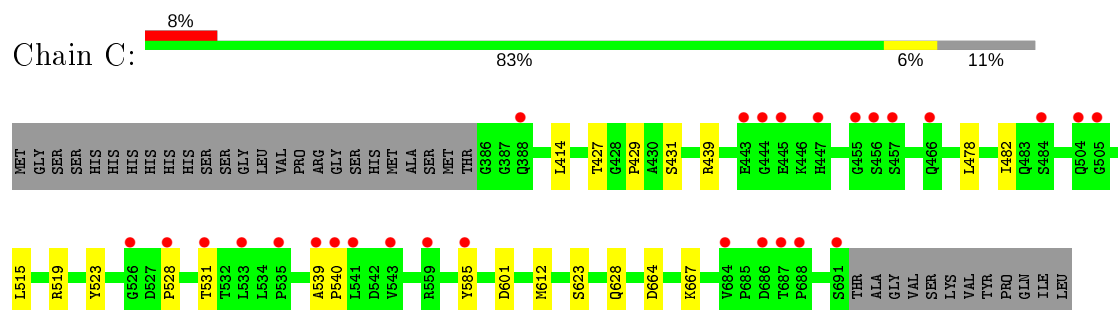
• Molecule 1: PUTATIVE FIBER PROTEIN



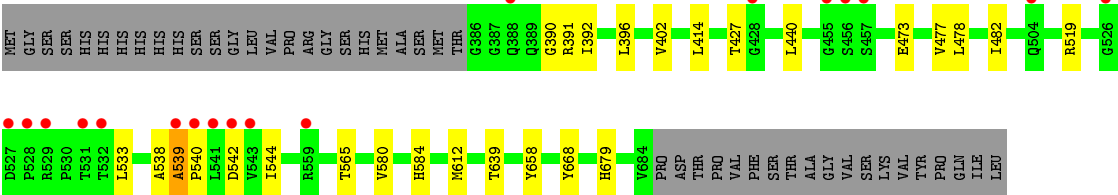
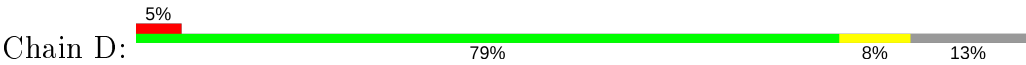
• Molecule 1: PUTATIVE FIBER PROTEIN



• Molecule 1: PUTATIVE FIBER PROTEIN



• Molecule 1: PUTATIVE FIBER PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.69Å 77.33Å 94.11Å 90.00° 101.45° 90.00°	Depositor
Resolution (Å)	35.00 – 1.90 34.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.6 (35.00-1.90) 95.6 (34.98-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.206 , 0.259 0.212 , 0.259	Depositor DCC
R_{free} test set	2124 reflections (2.39%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 62.5	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	0.97	EDS
Total number of atoms	10265	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 84.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5445e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.51	0/2434	0.64	0/3331
1	B	0.56	0/2477	0.65	0/3391
1	C	0.52	0/2490	0.64	0/3409
1	D	0.50	0/2428	0.64	0/3322
All	All	0.53	0/9829	0.64	0/13453

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2366	0	2358	26	0
1	B	2408	0	2401	24	0
1	C	2420	0	2402	13	0
1	D	2362	0	2359	21	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
2	C	12	0	16	0	0
2	D	6	0	8	0	0
3	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	0	0	0
3	C	12	0	0	0	0
3	D	12	0	0	0	0
4	A	155	0	0	1	0
4	B	168	0	0	2	0
4	C	160	0	0	2	0
4	D	142	0	0	2	0
All	All	10265	0	9568	83	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 (83) 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:539:ALA:CB	1:A:542:ASP:HB2	1.97	0.94
1:A:539:ALA:HB1	1:A:542:ASP:HB2	1.46	0.93
1:C:528:PRO:O	1:C:531:THR:HG22	1.77	0.84
1:D:539:ALA:HB3	1:D:542:ASP:HB2	1.61	0.81
1:B:538:ALA:O	1:B:542:ASP:OD2	1.99	0.80
1:A:539:ALA:HB1	1:A:540:PRO:CD	2.16	0.75
1:B:612:MET:HE3	4:B:2110:HOH:O	1.89	0.73
1:D:539:ALA:HB1	1:D:540:PRO:CD	2.24	0.68
1:A:538:ALA:O	1:A:539:ALA:HB2	1.93	0.67
1:D:539:ALA:HB1	1:D:540:PRO:HD2	1.78	0.65
1:B:478[B]:LEU:HD23	1:B:478[B]:LEU:C	2.18	0.63
1:A:552:LEU:HD13	1:A:556:LEU:HD13	1.80	0.63
1:B:390:GLY:O	1:B:519:ARG:NH1	2.33	0.61
1:D:402:VAL:HG11	1:D:482:ILE:HG13	1.82	0.60
1:A:439:ARG:HB3	1:A:585[B]:TYR:CD2	2.36	0.60
1:B:539:ALA:HB1	1:B:540:PRO:HD2	1.83	0.59
1:D:478[B]:LEU:HD23	1:D:478[B]:LEU:C	2.23	0.59
1:A:539:ALA:HB1	1:A:540:PRO:HD2	1.83	0.58
1:A:612:MET:HE3	4:A:2101:HOH:O	2.02	0.58
1:C:427:THR:HG23	1:C:431:SER:HB2	1.86	0.57
1:A:439:ARG:HD3	1:A:585[B]:TYR:CD1	2.39	0.57
1:D:477:VAL:HG11	1:D:533:LEU:HB3	1.87	0.56
1:C:414:LEU:HD23	1:C:515:LEU:HD23	1.88	0.56
1:D:538:ALA:O	1:D:539:ALA:CB	2.54	0.56
1:A:454:GLU:HG3	1:A:503:LEU:HD21	1.88	0.56
1:A:538:ALA:O	1:A:539:ALA:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ARG:HD2	4:C:2001:HOH:O	2.07	0.55
1:B:482:ILE:HG22	1:B:482:ILE:O	2.07	0.54
1:A:539:ALA:CB	1:A:540:PRO:CD	2.86	0.53
1:C:664:ASP:O	1:C:667:LYS:HE3	2.10	0.52
1:A:478:LEU:C	1:A:478:LEU:HD23	2.30	0.52
1:D:612:MET:HE2	4:D:2100:HOH:O	2.10	0.51
1:B:580:VAL:HG12	1:B:590:VAL:HG22	1.92	0.51
1:C:601:ASP:O	1:C:628:GLN:HA	2.11	0.51
1:D:390:GLY:O	1:D:519:ARG:NH1	2.43	0.51
1:C:612:MET:HE2	4:C:2110:HOH:O	2.10	0.50
1:B:402:VAL:CG1	1:B:406:ALA:HB3	2.41	0.50
1:D:580:VAL:HG23	1:D:668:TYR:HB2	1.94	0.50
1:D:427:THR:HG23	1:D:427:THR:O	2.12	0.50
1:C:439:ARG:HB3	1:C:585[A]:TYR:CD2	2.47	0.50
1:B:427:THR:HG23	1:B:505:GLY:O	2.12	0.50
1:B:449:VAL:HG13	1:B:462:GLU:HG3	1.94	0.49
1:A:664:ASP:O	1:A:667:LYS:HE3	2.14	0.48
1:A:449:VAL:HG13	1:A:462:GLU:CG	2.44	0.47
1:B:538:ALA:O	1:B:539:ALA:HB3	2.14	0.47
1:B:454:GLU:HG2	1:B:503:LEU:HD21	1.96	0.47
1:D:539:ALA:CB	1:D:540:PRO:CD	2.93	0.47
1:D:565[A]:THR:HG22	1:D:679:HIS:HB3	1.96	0.46
1:A:529:ARG:HB3	1:A:530:PRO:HD3	1.97	0.46
1:A:414:LEU:HD23	1:A:515:LEU:HD23	1.98	0.46
1:A:552:LEU:HD13	1:A:556:LEU:CD1	2.44	0.46
1:C:523:TYR:CE1	1:D:391:ARG:HD3	2.50	0.46
1:A:427:THR:HG23	1:A:431:SER:HB2	1.97	0.45
1:A:600:SER:OG	1:A:603:LYS:HB2	2.16	0.45
1:A:441:PRO:HD2	1:A:446:LYS:HA	1.98	0.45
1:B:639:THR:HG23	1:B:658:TYR:OH	2.17	0.45
1:D:539:ALA:HB3	1:D:542:ASP:CB	2.41	0.45
1:B:402:VAL:HG13	1:B:406:ALA:HB3	1.99	0.45
1:C:439:ARG:HD3	1:C:585[A]:TYR:CE1	2.52	0.44
1:D:584:HIS:HB3	4:D:2082:HOH:O	2.17	0.44
1:B:601:ASP:OD1	1:B:629:ARG:HD2	2.18	0.44
1:C:482:ILE:N	1:C:482:ILE:HD13	2.33	0.43
1:B:539:ALA:HB3	1:B:542:ASP:OD2	2.18	0.43
1:A:473:GLU:HB3	1:A:544:ILE:HD12	2.01	0.42
1:A:449:VAL:HG13	1:A:462:GLU:HG2	2.01	0.42
1:B:529:ARG:N	1:B:530:PRO:CD	2.82	0.42
1:D:538:ALA:O	1:D:539:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLU:CG	1:A:503:LEU:HD21	2.50	0.42
1:D:414:LEU:HD13	1:D:440:LEU:HD11	2.01	0.42
1:D:639:THR:HG23	1:D:658:TYR:OH	2.19	0.42
1:C:539:ALA:HB1	1:C:540:PRO:CD	2.49	0.42
1:D:392:ILE:HD13	1:D:396:LEU:HD13	2.01	0.42
1:B:597:GLY:O	1:B:604:GLY:HA3	2.20	0.42
1:D:473:GLU:HA	1:D:544:ILE:HD13	2.01	0.42
1:B:558:PRO:HA	1:B:639:THR:HG22	2.00	0.41
1:A:402:VAL:HG11	1:A:482:ILE:HG13	2.03	0.41
1:B:487:TYR:OH	4:B:2043:HOH:O	2.20	0.41
1:B:472:ARG:C	1:B:473:GLU:HG3	2.40	0.41
1:B:413:THR:HG21	1:B:544:ILE:HD12	2.01	0.41
1:B:529:ARG:O	1:B:532:THR:HG22	2.21	0.41
1:A:427:THR:O	1:A:427:THR:HG23	2.20	0.41
1:C:478:LEU:HD23	1:C:478:LEU:C	2.42	0.41
1:B:569:THR:HB	1:B:570:PRO:CD	2.51	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	299/343 (87%)	285 (95%)	11 (4%)	3 (1%)	15	6
1	B	305/343 (89%)	295 (97%)	9 (3%)	1 (0%)	41	31
1	C	306/343 (89%)	293 (96%)	12 (4%)	1 (0%)	41	31
1	D	299/343 (87%)	288 (96%)	10 (3%)	1 (0%)	41	31
All	All	1209/1372 (88%)	1161 (96%)	42 (4%)	6 (0%)	29	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	PRO
1	A	539	ALA
1	D	539	ALA
1	A	540	PRO
1	C	429	PRO
1	B	539	ALA

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	266/302 (88%)	263 (99%)	3 (1%)	73	73
1	B	272/302 (90%)	271 (100%)	1 (0%)	91	91
1	C	273/302 (90%)	272 (100%)	1 (0%)	91	91
1	D	266/302 (88%)	266 (100%)	0	100	100
All	All	1077/1208 (89%)	1072 (100%)	5 (0%)	88	89

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

Mol	Chain	Res	Type
1	A	440	LEU
1	A	556	LEU
1	A	655	GLN
1	B	541	LEU
1	C	623	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	C	1692	-	5,5,5	0.34	0	5,5,5	0.20	0
3	NO3	A	1689	-	1,3,3	3.74	1 (100%)	0,3,3	0.00	-
2	GOL	B	1692	-	5,5,5	0.31	0	5,5,5	0.36	0
2	GOL	D	1685	-	5,5,5	0.29	0	5,5,5	0.28	0
3	NO3	C	1696	-	1,3,3	3.64	1 (100%)	0,3,3	0.00	-
3	NO3	A	1688	-	1,3,3	3.35	1 (100%)	0,3,3	0.00	-
2	GOL	C	1693	-	5,5,5	0.42	0	5,5,5	0.16	0
3	NO3	D	1687	-	1,3,3	3.34	1 (100%)	0,3,3	0.00	-
3	NO3	B	1694	-	1,3,3	3.46	1 (100%)	0,3,3	0.00	-
3	NO3	C	1694	-	1,3,3	3.41	1 (100%)	0,3,3	0.00	-
3	NO3	B	1695	-	1,3,3	3.52	1 (100%)	0,3,3	0.00	-
3	NO3	B	1696	-	1,3,3	3.66	1 (100%)	0,3,3	0.00	-
2	GOL	B	1693	-	5,5,5	0.47	0	5,5,5	0.55	0
3	NO3	A	1687	-	1,3,3	3.71	1 (100%)	0,3,3	0.00	-
2	GOL	A	1686	-	5,5,5	0.30	0	5,5,5	0.29	0
3	NO3	D	1688	-	1,3,3	3.73	1 (100%)	0,3,3	0.00	-
3	NO3	D	1686	-	1,3,3	3.71	1 (100%)	0,3,3	0.00	-
3	NO3	C	1695	-	1,3,3	3.43	1 (100%)	0,3,3	0.00	-

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	C	1692	-	-	2/4/4/4	-
2	GOL	B	1692	-	-	0/4/4/4	-
2	GOL	D	1685	-	-	0/4/4/4	-
2	GOL	C	1693	-	-	1/4/4/4	-
2	GOL	B	1693	-	-	2/4/4/4	-
2	GOL	A	1686	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1689	NO3	O1-N	3.74	1.41	1.24
3	D	1688	NO3	O1-N	3.73	1.41	1.24
3	D	1686	NO3	O1-N	3.71	1.41	1.24
3	A	1687	NO3	O1-N	3.71	1.41	1.24
3	B	1696	NO3	O1-N	3.66	1.40	1.24
3	C	1696	NO3	O1-N	3.64	1.40	1.24
3	B	1695	NO3	O1-N	3.52	1.40	1.24
3	B	1694	NO3	O1-N	3.46	1.40	1.24
3	C	1695	NO3	O1-N	3.43	1.39	1.24
3	C	1694	NO3	O1-N	3.41	1.39	1.24
3	A	1688	NO3	O1-N	3.35	1.39	1.24
3	D	1687	NO3	O1-N	3.34	1.39	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1692	GOL	O1-C1-C2-C3
2	B	1693	GOL	C1-C2-C3-O3
2	B	1693	GOL	O2-C2-C3-O3
2	C	1693	GOL	O1-C1-C2-C3
2	C	1692	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	300/343 (87%)	0.29	29 (9%) 7 9	13, 35, 81, 118	0
1	B	306/343 (89%)	0.41	31 (10%) 7 8	10, 30, 81, 122	0
1	C	306/343 (89%)	0.33	28 (9%) 9 10	12, 34, 88, 169	0
1	D	299/343 (87%)	0.23	18 (6%) 21 24	10, 36, 79, 119	0
All	All	1211/1372 (88%)	0.32	106 (8%) 10 11	10, 34, 81, 169	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	541	LEU	11.4
1	A	540	PRO	10.9
1	B	540	PRO	10.7
1	D	540	PRO	10.3
1	D	539	ALA	10.2
1	D	541	LEU	9.7
1	A	541	LEU	9.3
1	C	541	LEU	8.6
1	B	539	ALA	8.0
1	B	528	PRO	7.3
1	C	540	PRO	7.0
1	B	687	THR	7.0
1	B	526	GLY	6.2
1	B	531	THR	5.9
1	B	543	VAL	5.8
1	B	691	SER	5.8
1	D	543	VAL	5.7
1	C	686	ASP	5.6
1	B	532	THR	5.1
1	A	528	PRO	4.8
1	D	528	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	542	ASP	4.7
1	B	456	SER	4.4
1	C	687	THR	4.4
1	C	456	SER	4.4
1	D	542	ASP	4.4
1	B	686	ASP	4.4
1	D	531	THR	4.3
1	A	445	GLU	4.2
1	A	543	VAL	4.1
1	B	527	ASP	4.1
1	C	528	PRO	4.0
1	B	559	ARG	3.9
1	A	539	ALA	3.9
1	C	531	THR	3.8
1	B	529	ARG	3.8
1	A	527	ASP	3.7
1	D	527	ASP	3.7
1	C	445	GLU	3.7
1	D	504	GLN	3.6
1	A	559	ARG	3.6
1	C	504	GLN	3.5
1	B	386	GLY	3.5
1	A	685	PRO	3.5
1	B	505	GLY	3.4
1	C	484	SER	3.4
1	C	539	ALA	3.4
1	A	531	THR	3.4
1	C	543	VAL	3.3
1	A	525	PRO	3.3
1	B	684	VAL	3.3
1	C	691	SER	3.3
1	C	505	GLY	3.2
1	A	455	GLY	3.2
1	C	457	SER	3.2
1	D	559	ARG	3.2
1	A	457	SER	3.2
1	D	456	SER	3.2
1	A	456	SER	3.2
1	C	559	ARG	3.1
1	A	532	THR	3.1
1	A	538	ALA	3.1
1	C	455	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	532	THR	3.0
1	B	484	SER	3.0
1	B	504	GLN	2.9
1	C	444	GLY	2.8
1	C	585[A]	TYR	2.7
1	A	484	SER	2.7
1	C	535	PRO	2.6
1	C	533	LEU	2.6
1	D	457	SER	2.5
1	B	404	THR	2.5
1	A	428	GLY	2.5
1	C	526	GLY	2.5
1	A	542	ASP	2.5
1	A	533	LEU	2.5
1	C	684	VAL	2.4
1	A	505	GLY	2.4
1	D	455	GLY	2.4
1	C	388	GLN	2.4
1	A	466	GLN	2.4
1	D	388	GLN	2.3
1	A	526	GLY	2.3
1	B	405	GLY	2.3
1	A	444	GLY	2.2
1	D	526	GLY	2.2
1	B	688	PRO	2.2
1	B	685	PRO	2.2
1	A	447	HIS	2.1
1	D	428	GLY	2.1
1	A	388	GLN	2.1
1	B	402	VAL	2.1
1	B	457	SER	2.1
1	B	403	PRO	2.1
1	A	641	GLU	2.1
1	C	443	GLU	2.1
1	B	530	PRO	2.1
1	A	495	PRO	2.1
1	B	427	THR	2.0
1	C	447	HIS	2.0
1	A	430	ALA	2.0
1	B	388	GLN	2.0
1	C	688	PRO	2.0
1	C	466	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	529	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 carbohydrates 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(\AA^2)	Q<0.9
2	GOL	C	1693	6/6	0.66	0.20	53,57,60,60	0
2	GOL	B	1692	6/6	0.79	0.14	38,51,54,56	0
2	GOL	B	1693	6/6	0.79	0.23	41,54,57,59	0
3	NO3	A	1689	4/4	0.82	0.24	55,59,60,63	0
2	GOL	A	1686	6/6	0.82	0.15	40,49,53,54	0
2	GOL	C	1692	6/6	0.84	0.12	47,56,57,58	0
3	NO3	C	1696	4/4	0.86	0.20	52,56,56,58	0
2	GOL	D	1685	6/6	0.88	0.12	38,43,47,53	0
3	NO3	D	1688	4/4	0.90	0.13	30,34,36,40	0
3	NO3	C	1695	4/4	0.91	0.15	25,35,37,42	0
3	NO3	B	1695	4/4	0.94	0.13	28,32,34,43	0
3	NO3	B	1696	4/4	0.94	0.10	30,31,33,37	0
3	NO3	A	1687	4/4	0.95	0.11	19,26,27,27	0
3	NO3	D	1686	4/4	0.95	0.09	18,24,29,30	0
3	NO3	A	1688	4/4	0.95	0.09	26,32,38,39	0
3	NO3	D	1687	4/4	0.97	0.09	28,31,33,38	0
3	NO3	B	1694	4/4	0.97	0.08	16,20,25,25	0
3	NO3	C	1694	4/4	0.98	0.08	15,22,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.