



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:21 AM UTC

PDB ID : 3TW0 / pdb_00003tw0
Title : Structural Analysis of Adhesive Tip pilin, GBS104 from Group B Streptococcus agalactiae
Authors : Krishnan, V.; Narayana, S.V.L.
Deposited on : 2011-09-21
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

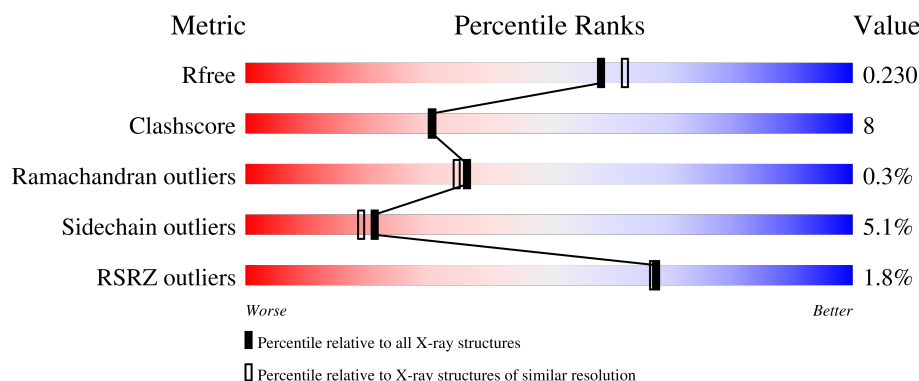
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	370	0% 80% 16% ..
1	B	370	2% 82% 14% ..
1	C	370	2% 77% 19% ..
1	D	370	3% 81% 13% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12159 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 Cell wall surface anchor family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2855	1795	483	570	7			
1	B	361	Total	C	N	O	S	0	0	0
			2855	1795	483	570	7			
1	C	360	Total	C	N	O	S	0	0	0
			2850	1792	482	569	7			
1	D	357	Total	C	N	O	S	0	0	0
			2820	1772	477	564	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	CYS	THR	engineered mutation	UNP Q8E0S5
A	571	CYS	LYS	engineered mutation	UNP Q8E0S5
B	564	CYS	THR	engineered mutation	UNP Q8E0S5
B	571	CYS	LYS	engineered mutation	UNP Q8E0S5
C	564	CYS	THR	engineered mutation	UNP Q8E0S5
C	571	CYS	LYS	engineered mutation	UNP Q8E0S5
D	564	CYS	THR	engineered mutation	UNP Q8E0S5
D	571	CYS	LYS	engineered mutation	UNP Q8E0S5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

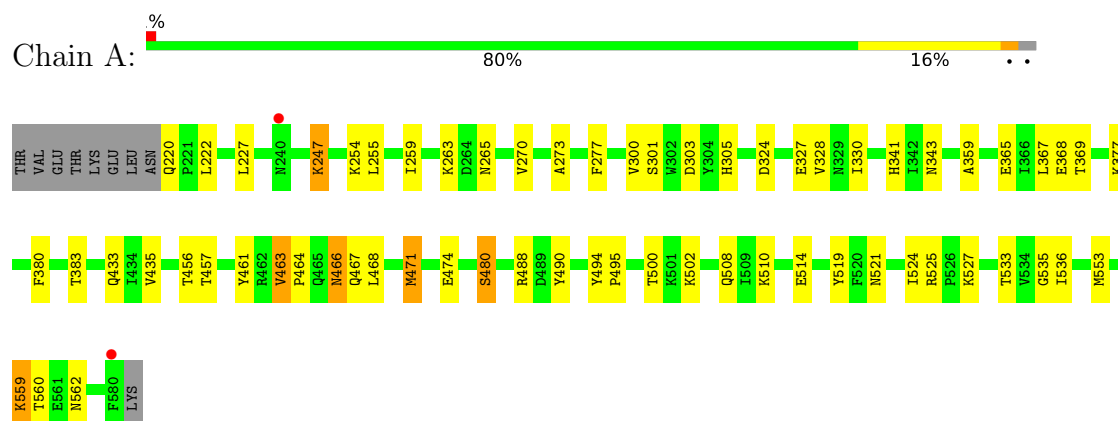
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	200	Total	O	0	0
			200	200		
4	B	197	Total	O	0	0
			197	197		
4	C	193	Total	O	0	0
			193	193		
4	D	169	Total	O	0	0
			169	169		

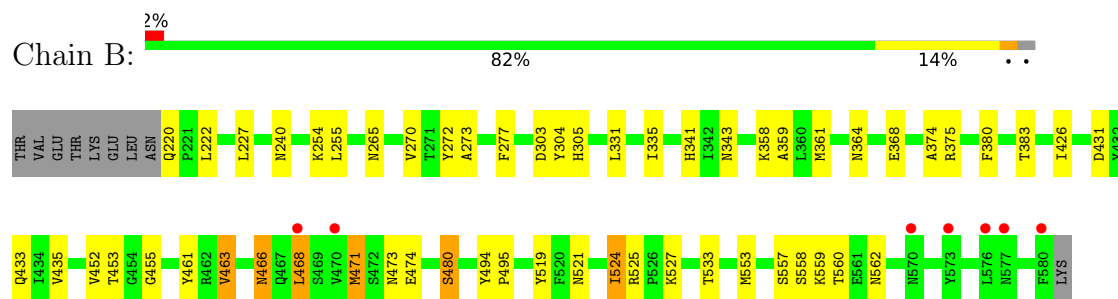
3 Residue-property plots

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.

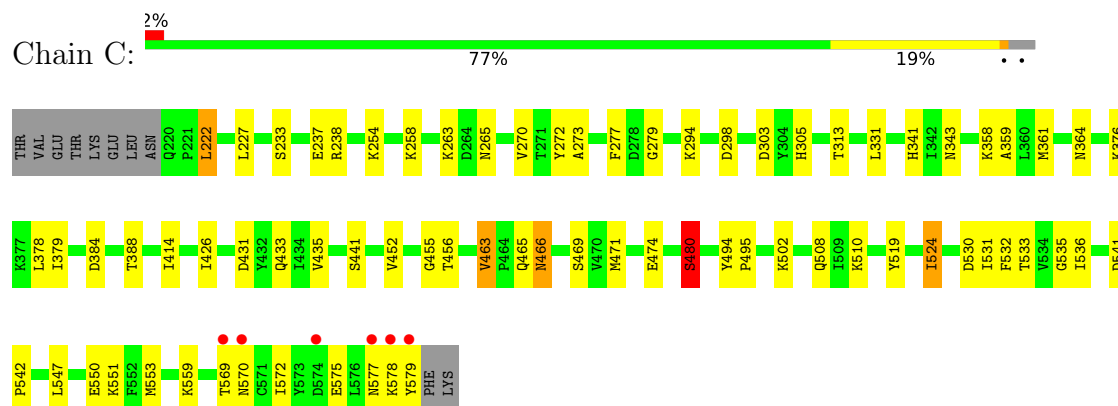
- Molecule 1: Cell wall surface anchor family protein



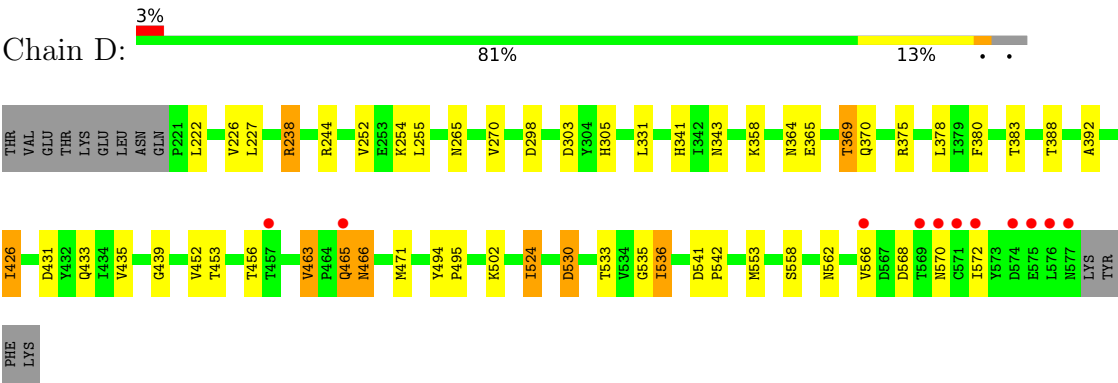
- Molecule 1: Cell wall surface anchor family protein



- Molecule 1: Cell wall surface anchor family protein



● Molecule 1: Cell wall surface anchor family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.07Å 77.26Å 96.40Å 74.12° 87.25° 89.99°	Depositor
Resolution (Å)	46.30 – 2.00 46.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (46.30-2.00) 89.0 (46.30-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.231 0.198 , 0.230	Depositor DCC
R_{free} test set	4418 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12159	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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: MG, ACT

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	0.82	0/2914	0.95	3/3955 (0.1%)
1	B	0.80	0/2914	0.96	4/3955 (0.1%)
1	C	0.81	0/2909	0.94	2/3948 (0.1%)
1	D	0.79	0/2878	0.92	1/3906 (0.0%)
All	All	0.80	0/11615	0.94	10/15764 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	ILE	CB-CA-C	-5.91	106.69	111.71
1	B	524	ILE	CB-CA-C	-5.62	106.94	111.71
1	B	335	ILE	CA-C-N	-5.59	114.49	120.03
1	B	335	ILE	C-N-CA	-5.59	114.49	120.03
1	D	524	ILE	CB-CA-C	-5.34	107.17	111.71
1	C	480	SER	N-CA-C	5.25	121.98	110.80
1	C	524	ILE	CB-CA-C	-5.23	107.27	111.71
1	B	480	SER	N-CA-C	5.19	121.86	110.80
1	A	514	GLU	CA-C-N	-5.03	113.75	119.28
1	A	514	GLU	C-N-CA	-5.03	113.75	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	SER	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	2855	0	2754	44	0
1	B	2855	0	2754	42	0
1	C	2850	0	2752	52	0
1	D	2820	0	2723	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
4	A	200	0	0	1	0
4	B	197	0	0	1	0
4	C	193	0	0	5	0
4	D	169	0	0	1	0
All	All	12159	0	10995	185	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 8.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:THR:HG23	1:D:553:MET:HE3	1.35	1.04
1:D:533:THR:HG22	1:D:553:MET:HE2	1.43	0.98
1:A:463:VAL:HB	1:A:471:MET:HE2	1.45	0.97
1:C:222:LEU:HD11	1:C:378:LEU:CD1	1.96	0.96
1:C:550:GLU:HB3	4:C:750:HOH:O	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:THR:HG22	1:B:553:MET:CE	1.98	0.93
1:C:341:HIS:HD2	1:C:343:ASN:H	1.15	0.93
1:C:463:VAL:HB	1:C:471:MET:CE	1.98	0.93
1:D:383:THR:CG2	1:D:553:MET:HE3	2.04	0.87
1:D:358:LYS:HE3	1:D:431:ASP:OD2	1.78	0.83
1:B:466:ASN:HD22	1:B:466:ASN:H	1.25	0.81
1:B:533:THR:HG22	1:B:553:MET:HE2	1.60	0.81
1:C:222:LEU:HD11	1:C:378:LEU:HD13	1.61	0.81
1:D:463:VAL:HB	1:D:471:MET:CE	2.11	0.80
1:A:463:VAL:HB	1:A:471:MET:CE	2.12	0.79
1:B:558:SER:HB2	1:B:562:ASN:HD22	1.45	0.78
1:C:533:THR:HG22	1:C:553:MET:CE	2.14	0.78
1:B:358:LYS:HE3	1:B:431:ASP:OD2	1.83	0.78
1:A:533:THR:HG22	1:A:553:MET:CE	2.15	0.77
1:C:533:THR:HG22	1:C:553:MET:HE2	1.66	0.77
1:A:533:THR:HG22	1:A:553:MET:HE2	1.66	0.76
1:C:341:HIS:CD2	1:C:343:ASN:H	2.01	0.76
1:D:222:LEU:HD11	1:D:378:LEU:HG	1.67	0.76
1:B:521:ASN:OD1	1:B:525:ARG:NH1	2.20	0.75
1:D:238:ARG:CG	1:D:238:ARG:HH11	2.00	0.75
1:C:222:LEU:H	1:C:265:ASN:ND2	1.85	0.75
1:C:535:GLY:HA2	1:C:553:MET:HE1	1.71	0.73
1:C:535:GLY:CA	1:C:553:MET:HE1	2.20	0.72
1:C:227:LEU:HD23	1:C:270:VAL:HB	1.72	0.71
1:A:222:LEU:H	1:A:265:ASN:ND2	1.87	0.71
1:B:303:ASP:OD2	1:B:305:HIS:HD2	1.74	0.71
1:B:533:THR:HG22	1:B:553:MET:HE3	1.73	0.70
1:C:463:VAL:HB	1:C:471:MET:HE3	1.73	0.70
1:A:255:LEU:HD22	1:A:380:PHE:CD2	2.28	0.69
1:A:559:LYS:HG2	1:A:562:ASN:ND2	2.08	0.69
1:B:341:HIS:CD2	1:B:343:ASN:H	2.10	0.69
1:D:222:LEU:H	1:D:265:ASN:ND2	1.92	0.68
1:B:364:ASN:HB2	1:B:524:ILE:CD1	2.25	0.67
1:B:341:HIS:HD2	1:B:343:ASN:H	1.43	0.67
1:D:341:HIS:HD2	1:D:343:ASN:H	1.43	0.66
1:D:392:ALA:HB3	1:D:426:ILE:HG13	1.78	0.65
1:D:238:ARG:HH11	1:D:238:ARG:HG3	1.62	0.65
1:D:494:TYR:HB2	1:D:495:PRO:HA	1.79	0.64
1:B:533:THR:CG2	1:B:553:MET:CE	2.75	0.64
1:D:533:THR:CG2	1:D:553:MET:HE2	2.24	0.64
1:B:452:VAL:HG23	1:B:455:GLY:HA3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:TYR:CE2	1:B:471:MET:HE1	2.31	0.64
1:A:535:GLY:HA2	1:A:553:MET:HE1	1.80	0.64
1:D:255:LEU:HD21	1:D:380:PHE:CG	2.32	0.64
1:C:222:LEU:H	1:C:265:ASN:HD22	1.44	0.63
1:A:222:LEU:H	1:A:265:ASN:HD22	1.46	0.63
1:C:494:TYR:HB2	1:C:495:PRO:HA	1.81	0.63
1:B:466:ASN:HD22	1:B:466:ASN:N	1.98	0.61
1:D:227:LEU:HD23	1:D:270:VAL:HB	1.82	0.61
1:D:303:ASP:OD2	1:D:305:HIS:HD2	1.83	0.61
1:C:222:LEU:CD1	1:C:378:LEU:CD1	2.75	0.61
1:B:303:ASP:OD2	1:B:305:HIS:CD2	2.53	0.61
1:C:341:HIS:HD2	1:C:343:ASN:N	1.94	0.60
1:A:500:THR:OG1	1:A:502:LYS:HD3	2.02	0.60
1:D:535:GLY:HA2	1:D:553:MET:HE1	1.83	0.59
1:B:368:GLU:OE2	1:B:527:LYS:HE3	2.03	0.59
1:D:378:LEU:HD22	1:D:530:ASP:HB3	1.85	0.58
1:C:361:MET:HG2	1:C:519:TYR:CZ	2.38	0.58
1:D:365:GLU:O	1:D:369:THR:HB	2.04	0.58
1:B:533:THR:CG2	1:B:553:MET:HE3	2.33	0.57
1:B:461:TYR:HE2	1:B:471:MET:HE1	1.68	0.57
1:C:222:LEU:CD1	1:C:378:LEU:HD13	2.34	0.57
1:C:508:GLN:HE21	1:C:510:LYS:HE3	1.68	0.57
1:C:508:GLN:NE2	1:C:510:LYS:HE3	2.20	0.57
1:A:368:GLU:OE2	1:A:527:LYS:HE3	2.06	0.56
1:C:466:ASN:ND2	1:C:466:ASN:H	2.03	0.56
1:C:533:THR:HG22	1:C:553:MET:HE3	1.87	0.56
1:B:227:LEU:HD23	1:B:270:VAL:HB	1.88	0.55
1:D:378:LEU:HD22	1:D:530:ASP:CB	2.36	0.55
1:B:558:SER:HB2	1:B:562:ASN:ND2	2.20	0.55
1:C:305:HIS:HE1	1:C:474:GLU:OE2	1.88	0.55
1:A:365:GLU:O	1:A:369:THR:OG1	2.20	0.55
1:C:364:ASN:HB2	1:C:524:ILE:HD12	1.88	0.55
1:A:494:TYR:HB2	1:A:495:PRO:HA	1.87	0.55
1:B:533:THR:CG2	1:B:553:MET:HE2	2.34	0.55
1:A:341:HIS:CD2	1:A:343:ASN:H	2.26	0.54
1:A:383:THR:HG23	1:A:553:MET:HE3	1.89	0.54
1:D:369:THR:HG22	1:D:370:GLN:HG3	1.90	0.54
1:A:227:LEU:HD23	1:A:270:VAL:HB	1.89	0.53
1:A:273:ALA:HB3	1:A:277:PHE:CZ	2.44	0.53
1:B:525:ARG:NH2	1:B:557:SER:O	2.42	0.53
1:D:536:ILE:HG13	1:D:566:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:HIS:HE1	1:A:474:GLU:OE2	1.92	0.52
1:A:341:HIS:HD2	1:A:343:ASN:H	1.56	0.52
1:C:532:PHE:HZ	1:C:575:GLU:HG2	1.73	0.52
1:A:255:LEU:HD22	1:A:380:PHE:CG	2.45	0.52
1:B:220:GLN:NE2	1:B:374:ALA:O	2.43	0.52
1:D:383:THR:HG23	1:D:553:MET:CE	2.24	0.52
1:C:361:MET:HG2	1:C:519:TYR:OH	2.09	0.52
1:D:558:SER:HB2	1:D:562:ASN:HD22	1.74	0.52
1:B:331:LEU:C	1:B:331:LEU:HD23	2.36	0.51
1:A:521:ASN:OD1	1:A:525:ARG:NH1	2.42	0.51
1:D:303:ASP:OD2	1:D:305:HIS:CD2	2.64	0.51
1:A:461:TYR:CE2	1:A:471:MET:HE1	2.45	0.51
1:A:467:GLN:HA	4:A:621:HOH:O	2.09	0.51
1:D:378:LEU:CD2	1:D:530:ASP:HB2	2.41	0.51
1:A:303:ASP:OD2	1:A:305:HIS:HD2	1.94	0.50
1:D:502:LYS:HD3	4:D:751:HOH:O	2.10	0.50
1:B:494:TYR:HB2	1:B:495:PRO:HA	1.93	0.50
1:C:578:LYS:H	1:C:579:TYR:HD1	1.59	0.50
1:B:305:HIS:HE1	1:B:474:GLU:OE2	1.95	0.50
1:D:364:ASN:HB2	1:D:524:ILE:HD12	1.94	0.50
1:A:466:ASN:H	1:A:466:ASN:HD22	1.60	0.50
1:B:222:LEU:H	1:B:265:ASN:ND2	2.10	0.50
1:C:237:GLU:OE2	1:C:341:HIS:HE1	1.95	0.50
1:B:255:LEU:HD22	1:B:380:PHE:CD2	2.47	0.50
1:B:453:THR:C	1:B:455:GLY:H	2.19	0.50
1:B:463:VAL:CG2	1:B:468:LEU:HD22	2.42	0.50
1:B:368:GLU:OE2	1:B:527:LYS:HD2	2.12	0.49
1:A:535:GLY:CA	1:A:553:MET:HE1	2.42	0.48
1:C:279:GLY:HA2	1:C:313:THR:O	2.14	0.48
1:C:547:LEU:HG	1:C:551:LYS:HE3	1.94	0.48
1:A:519:TYR:CD2	1:A:519:TYR:C	2.91	0.48
1:B:272:TYR:CG	1:B:359:ALA:HB2	2.49	0.48
1:B:473:ASN:ND2	4:B:814:HOH:O	2.47	0.47
1:A:533:THR:HG22	1:A:553:MET:HE3	1.94	0.47
1:D:226:VAL:HG11	1:D:252:VAL:HG13	1.96	0.47
1:D:463:VAL:HB	1:D:471:MET:HE1	1.95	0.47
1:C:569:THR:HA	1:C:572:ILE:HD12	1.97	0.47
1:C:502:LYS:NZ	4:C:187:HOH:O	2.48	0.47
1:D:255:LEU:HD21	1:D:380:PHE:CB	2.44	0.47
1:B:463:VAL:HB	1:B:471:MET:HE2	1.96	0.47
1:C:463:VAL:HB	1:C:471:MET:HE1	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ASN:H	1:A:466:ASN:ND2	2.13	0.46
1:A:508:GLN:HE21	1:A:510:LYS:HE3	1.79	0.46
1:B:361:MET:HG2	1:B:519:TYR:CZ	2.49	0.46
1:D:466:ASN:HD22	1:D:466:ASN:N	2.13	0.46
1:A:247:LYS:HB3	1:A:247:LYS:HE3	1.86	0.46
1:D:244:ARG:HG2	1:D:536:ILE:HG22	1.97	0.46
1:B:222:LEU:H	1:B:265:ASN:HD22	1.61	0.46
1:A:383:THR:CG2	1:A:553:MET:HE3	2.45	0.46
1:A:508:GLN:NE2	1:A:510:LYS:HE3	2.30	0.46
1:C:480:SER:HA	4:C:121:HOH:O	2.16	0.46
1:C:535:GLY:N	1:C:553:MET:HE1	2.31	0.46
1:A:559:LYS:NZ	1:A:562:ASN:HD21	2.14	0.46
1:C:294:LYS:HE3	4:C:766:HOH:O	2.16	0.45
1:D:463:VAL:HB	1:D:471:MET:HE3	1.95	0.45
1:B:273:ALA:HB3	1:B:277:PHE:CZ	2.51	0.45
1:C:222:LEU:HD11	1:C:378:LEU:HD11	1.89	0.45
1:D:341:HIS:CD2	1:D:343:ASN:H	2.29	0.45
1:C:331:LEU:C	1:C:331:LEU:HD23	2.41	0.45
1:C:358:LYS:HE2	1:C:431:ASP:OD2	2.17	0.45
1:D:238:ARG:HH11	1:D:238:ARG:HG2	1.81	0.45
1:A:463:VAL:HA	1:A:464:PRO:HD3	1.90	0.45
1:A:367:LEU:HD22	1:A:377:LYS:HB3	1.99	0.44
1:B:240:ASN:O	1:B:240:ASN:CG	2.60	0.44
1:D:238:ARG:HG3	1:D:238:ARG:NH1	2.31	0.43
1:D:558:SER:HB2	1:D:562:ASN:ND2	2.33	0.43
1:A:324:ASP:O	1:A:328:VAL:HG23	2.17	0.43
1:D:244:ARG:HA	1:D:536:ILE:CG2	2.48	0.43
1:D:502:LYS:HB3	1:D:502:LYS:HE3	1.78	0.43
1:D:533:THR:HG22	1:D:553:MET:CE	2.32	0.43
1:A:533:THR:CG2	1:A:553:MET:HE2	2.44	0.42
1:C:378:LEU:HG	1:C:530:ASP:HB2	2.00	0.42
1:C:541:ASP:HA	1:C:542:PRO:HA	1.93	0.42
1:A:255:LEU:HG	1:A:259:ILE:HD11	2.02	0.42
1:A:303:ASP:OD2	1:A:305:HIS:CD2	2.72	0.42
1:C:303:ASP:OD2	1:C:305:HIS:HD2	2.02	0.42
1:D:388:THR:OG1	1:D:439:GLY:HA2	2.18	0.42
1:D:331:LEU:C	1:D:331:LEU:HD23	2.45	0.42
1:A:327:GLU:HA	1:A:330:ILE:HD12	2.02	0.42
1:C:379:ILE:HB	1:C:531:ILE:HG12	2.01	0.42
1:D:541:ASP:HA	1:D:542:PRO:HA	1.90	0.42
1:C:541:ASP:HB2	4:C:812:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HG	1:A:259:ILE:CD1	2.50	0.41
1:B:383:THR:CG2	1:B:553:MET:HE3	2.50	0.41
1:C:361:MET:CG	1:C:519:TYR:CZ	3.03	0.41
1:C:273:ALA:HB3	1:C:277:PHE:CZ	2.56	0.41
1:C:463:VAL:CB	1:C:471:MET:CE	2.85	0.41
1:D:568:ASP:OD1	1:D:570:ASN:HB2	2.20	0.41
1:B:304:TYR:CZ	1:B:305:HIS:NE2	2.89	0.41
1:C:272:TYR:CG	1:C:359:ALA:HB2	2.55	0.41
1:C:388:THR:HG22	1:C:441:SER:C	2.45	0.41
1:A:488:ARG:HD3	1:A:490:TYR:OH	2.20	0.41
1:B:466:ASN:N	1:B:466:ASN:ND2	2.65	0.41
1:C:233:SER:OG	1:C:384:ASP:OD2	2.39	0.41
1:D:227:LEU:CD2	1:D:270:VAL:HB	2.50	0.41
1:D:465:GLN:HE21	1:D:465:GLN:HB3	1.68	0.40
1:C:233:SER:HA	1:C:238:ARG:HD2	2.03	0.40
1:A:227:LEU:HD22	1:A:359:ALA:HB1	2.03	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	359/370 (97%)	348 (97%)	10 (3%)	1 (0%)	36	35
1	B	359/370 (97%)	346 (96%)	12 (3%)	1 (0%)	36	35
1	C	358/370 (97%)	343 (96%)	12 (3%)	3 (1%)	16	11
1	D	355/370 (96%)	339 (96%)	16 (4%)	0	100	100
All	All	1431/1480 (97%)	1376 (96%)	50 (4%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	480	SER
1	C	455	GLY
1	C	480	SER
1	A	480	SER
1	C	577	ASN

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	315/325 (97%)	298 (95%)	17 (5%)	20	17
1	B	315/325 (97%)	304 (96%)	11 (4%)	32	32
1	C	315/325 (97%)	296 (94%)	19 (6%)	17	14
1	D	312/325 (96%)	295 (95%)	17 (5%)	20	17
All	All	1257/1300 (97%)	1193 (95%)	64 (5%)	21	19

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	247	LYS
1	A	254	LYS
1	A	263	LYS
1	A	300	VAL
1	A	301	SER
1	A	433	GLN
1	A	435	VAL
1	A	456	THR
1	A	457	THR
1	A	463	VAL
1	A	466	ASN
1	A	468	LEU
1	A	471	MET
1	A	536	ILE
1	A	559	LYS
1	A	560	THR

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Mol	Chain	Res	Type
1	B	254	LYS
1	B	375	ARG
1	B	426	ILE
1	B	433	GLN
1	B	435	VAL
1	B	463	VAL
1	B	466	ASN
1	B	468	LEU
1	B	471	MET
1	B	559	LYS
1	B	560	THR
1	C	222	LEU
1	C	254	LYS
1	C	258	LYS
1	C	263	LYS
1	C	298	ASP
1	C	376	LYS
1	C	414	ILE
1	C	426	ILE
1	C	433	GLN
1	C	435	VAL
1	C	452	VAL
1	C	456	THR
1	C	463	VAL
1	C	465	GLN
1	C	466	ASN
1	C	469	SER
1	C	536	ILE
1	C	559	LYS
1	C	570	ASN
1	D	238	ARG
1	D	254	LYS
1	D	298	ASP
1	D	369	THR
1	D	375	ARG
1	D	426	ILE
1	D	433	GLN
1	D	435	VAL
1	D	452	VAL
1	D	453	THR
1	D	456	THR
1	D	463	VAL

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Mol	Chain	Res	Type
1	D	465	GLN
1	D	466	ASN
1	D	530	ASP
1	D	536	ILE
1	D	572	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	305	HIS
1	A	314	HIS
1	A	341	HIS
1	A	364	ASN
1	A	404	GLN
1	A	465	GLN
1	A	466	ASN
1	A	467	GLN
1	A	508	GLN
1	A	562	ASN
1	B	265	ASN
1	B	305	HIS
1	B	314	HIS
1	B	341	HIS
1	B	343	ASN
1	B	350	GLN
1	B	364	ASN
1	B	404	GLN
1	B	466	ASN
1	B	562	ASN
1	C	265	ASN
1	C	305	HIS
1	C	341	HIS
1	C	343	ASN
1	C	350	GLN
1	C	404	GLN
1	C	465	GLN
1	C	466	ASN
1	C	467	GLN
1	C	508	GLN
1	D	240	ASN
1	D	265	ASN

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Mol	Chain	Res	Type
1	D	305	HIS
1	D	314	HIS
1	D	326	ASN
1	D	341	HIS
1	D	465	GLN
1	D	466	ASN
1	D	473	ASN
1	D	565	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ACT	B	702	2	3,3,3	0.97	0	3,3,3	1.55	1 (33%)
3	ACT	C	702	2	3,3,3	0.80	0	3,3,3	1.56	1 (33%)
3	ACT	A	702	2	3,3,3	0.90	0	3,3,3	1.59	1 (33%)
3	ACT	D	702	2	3,3,3	0.71	0	3,3,3	1.52	1 (33%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	702	ACT	OXT-C-CH3	2.11	123.89	115.05
3	A	702	ACT	OXT-C-O	-2.08	114.32	122.03
3	D	702	ACT	OXT-C-CH3	2.03	123.57	115.05
3	B	702	ACT	OXT-C-CH3	2.01	123.47	115.05

There are no chirality outliers.

There are no torsion outliers.

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, 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	361/370 (97%)	-0.15	2 (0%) 85 85	12, 22, 40, 54	0
1	B	361/370 (97%)	-0.05	7 (1%) 66 66	12, 23, 43, 63	0
1	C	360/370 (97%)	-0.16	6 (1%) 69 68	12, 21, 44, 52	0
1	D	357/370 (96%)	0.01	11 (3%) 51 50	12, 24, 46, 70	0
All	All	1439/1480 (97%)	-0.09	26 (1%) 67 67	12, 22, 43, 70	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	580	PHE	4.4
1	A	580	PHE	4.2
1	D	572	ILE	4.1
1	D	576	LEU	3.6
1	B	577	ASN	3.4
1	C	569	THR	3.4
1	D	577	ASN	3.3
1	C	579	TYR	3.2
1	C	570	ASN	2.9
1	C	578	LYS	2.8
1	D	570	ASN	2.7
1	D	566	VAL	2.7
1	D	575	GLU	2.7
1	D	571	CYS	2.7
1	B	576	LEU	2.7
1	D	569	THR	2.7
1	C	574	ASP	2.5
1	D	574	ASP	2.4
1	B	573	TYR	2.3
1	D	465	GLN	2.3
1	B	570	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	468	LEU	2.1
1	B	470	VAL	2.1
1	A	240	ASN	2.0
1	D	457	THR	2.0
1	C	577	ASN	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
3	ACT	B	702	4/4	0.91	0.10	16,16,16,18	0
3	ACT	D	702	4/4	0.91	0.09	21,22,22,22	0
3	ACT	C	702	4/4	0.92	0.13	16,17,17,17	0
3	ACT	A	702	4/4	0.97	0.06	15,16,17,17	0
2	MG	A	701	1/1	0.98	0.03	20,20,20,20	0
2	MG	B	701	1/1	0.98	0.05	20,20,20,20	0
2	MG	C	701	1/1	0.98	0.03	18,18,18,18	0
2	MG	D	701	1/1	0.98	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.