Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:25 PM GMT

PDB ID	:	3TW0
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

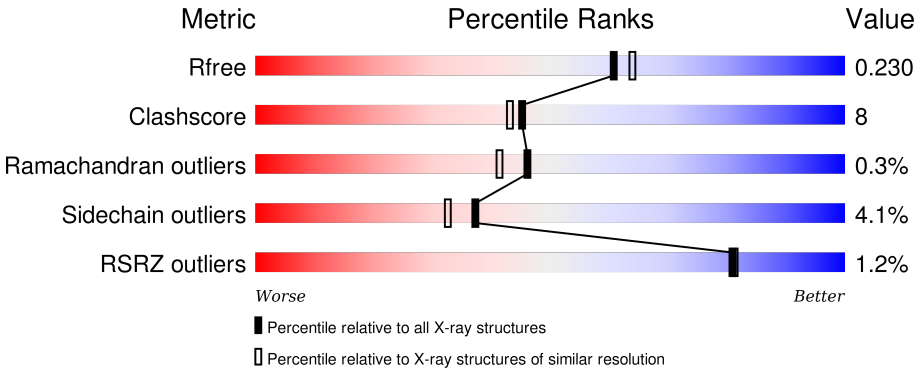
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	370	82% 14%
1	B	370	84% 13%
1	C	370	78% 18%
1	D	370	82% 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			

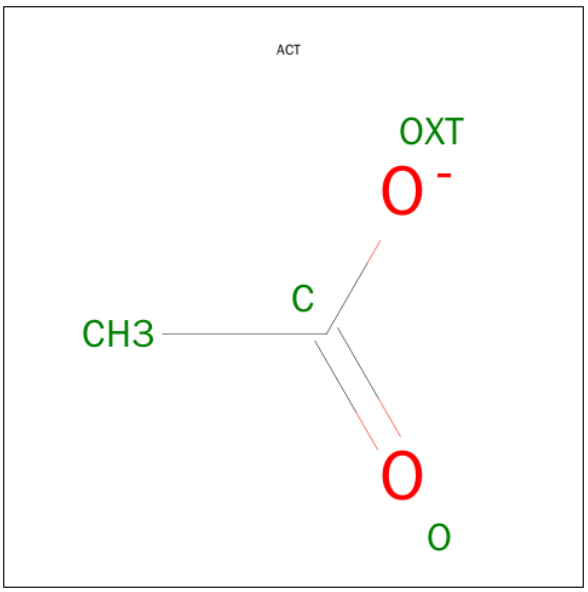
There are 8 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is water.

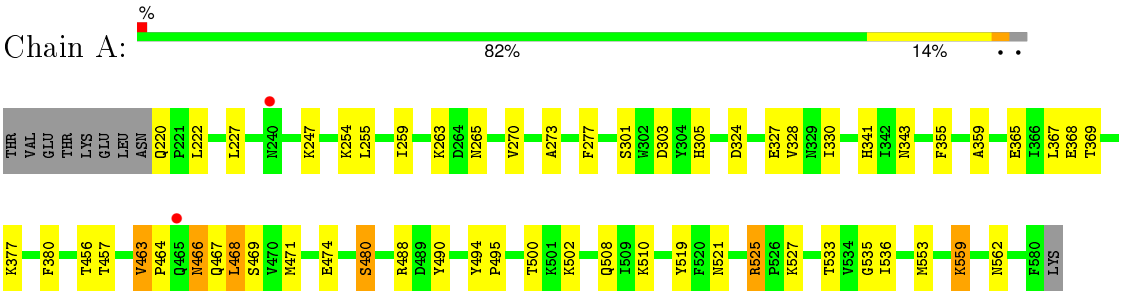
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	197	Total O 197 197	0	0
4	C	193	Total O 193 193	0	0
4	D	169	Total O 169 169	0	0

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 errors 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.

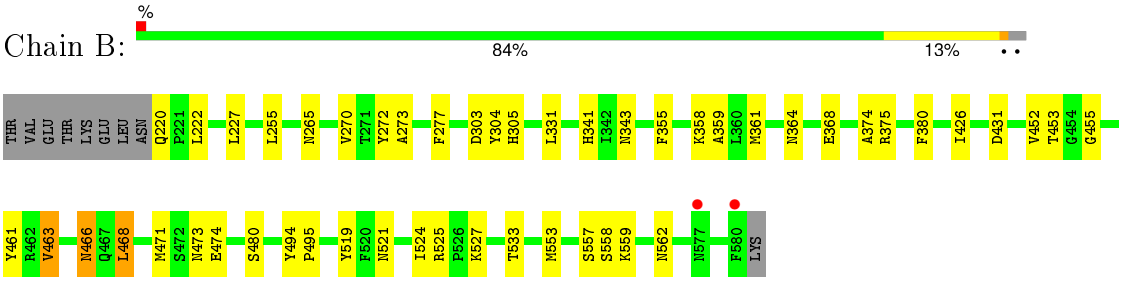
- Molecule 1: Cell wall surface anchor family protein

Chain A:



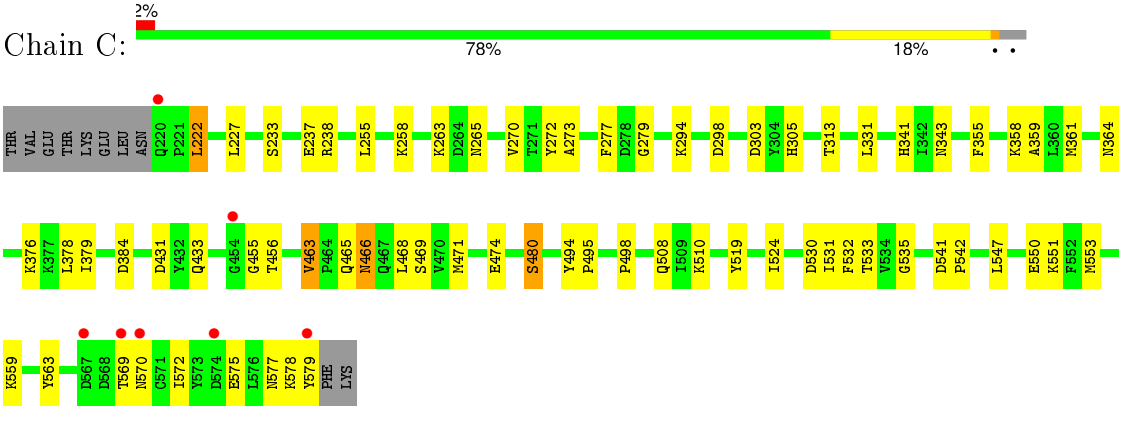
- Molecule 1: Cell wall surface anchor family protein

Chain B:



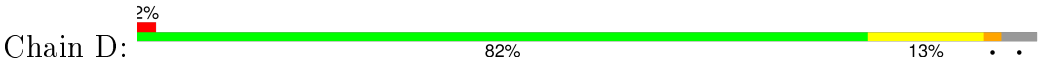
- Molecule 1: Cell wall surface anchor family protein

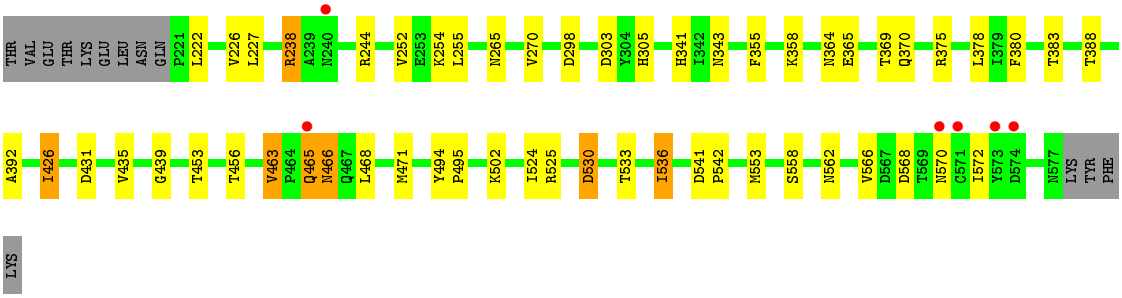
Chain C:



- Molecule 1: Cell wall surface anchor family protein

Chain D:




THR VAL GLU THR LYS GLU LEU ASN GLN P221 L222 V226 L227 R238 A239 N240 R244 V252 E253 K254 L255 N265 V270 D298 D303 Y304 H305 H341 I342 N343 F355 K358 N364 E365 T369 Q370 R375 L378 I379 F380 T383 T388
A392 I426 D431 V435 G439 T453 T456 V463 P464 Q465 N466 Q467 L468 M471 Y494 P495 K502 I524 R525 D530 T533 I536 D541 P542 M553 S558 N562 V566 D567 D568 T569 N570 C571 I572 Y573 D574 N577 LYS TYR PHE
LYS

4 Data and refinement statistics (i)

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) 80.7 (46.30-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.26%)	DCC
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 , 45.6	EDS
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 88442 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.67	0/2914	0.70	1/3955 (0.0%)
1	B	0.64	0/2914	0.70	0/3955
1	C	0.67	0/2909	0.73	2/3948 (0.1%)
1	D	0.63	0/2878	0.68	1/3906 (0.0%)
All	All	0.65	0/11615	0.70	4/15764 (0.0%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	468	LEU	CA-CB-CG	5.63	128.25	115.30
1	C	468	LEU	CA-CB-CG	5.47	127.88	115.30
1	D	468	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	255	LEU	CA-CB-CG	5.19	127.23	115.30

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 (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	2855	0	2754	40	0
1	B	2855	0	2754	38	0
1	C	2850	0	2752	51	0
1	D	2820	0	2723	46	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	4	0
4	D	169	0	0	1	0
All	All	12159	0	10995	175	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 (175) 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: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
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:C:533:THR:HG22	1:C:553:MET:HE3	1.52	0.92
1:A:533:THR:HG22	1:A:553:MET:HE3	1.56	0.87
1:A:463:VAL:HB	1:A:471:MET:HE2	1.59	0.83
1:D:358:LYS:HE3	1:D:431:ASP:OD2	1.78	0.83
1:B:466:ASN:H	1:B:466:ASN:HD22	1.25	0.81
1:C:222:LEU:HD11	1:C:378:LEU:HD13	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:THR:HG22	1:B:553:MET:HE3	1.63	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: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:HH11	1:D:238:ARG:CG	2.00	0.75
1:C:222:LEU:H	1:C:265:ASN:ND2	1.85	0.75
1:A:533:THR:CG2	1:A:553:MET:HE3	2.20	0.72
1:B:533:THR:HG22	1:B:553:MET:HE2	1.70	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:CG2	1:B:553:MET:HE3	2.21	0.71
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:C:463:VAL:HB	1:C:471:MET:HE3	1.73	0.68
1:D:222:LEU:H	1:D:265:ASN:ND2	1.92	0.68
1:D:383:THR:HG23	1:D:553:MET:CE	2.24	0.67
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:C:535:GLY:HA2	1:C:553:MET:HE1	1.75	0.67
1:D:341:HIS:HD2	1:D:343:ASN:H	1.43	0.66
1:C:533:THR:CG2	1:C:553:MET:HE3	2.25	0.66
1:D:392:ALA:HB3	1:D:426:ILE:HG13	1.78	0.65
1:D:238:ARG:HG3	1:D:238:ARG:HH11	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:B:452:VAL:HG23	1:B:455:GLY:HA3	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:N	1:B:466:ASN:HD22	1.98	0.61
1:D:383:THR:HG23	1:D:553:MET:HE1	1.81	0.61
1:D:227:LEU:HD23	1:D:270:VAL:HB	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:533:THR:HG22	1:D:553:MET:CE	2.32	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:D:533:THR:CG2	1:D:553:MET:HE3	2.34	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: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:466:ASN:H	1:C:466:ASN:ND2	2.03	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: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:D:533:THR:HG22	1:D:553:MET:HE3	1.88	0.54
1:A:341:HIS:CD2	1:A:343:ASN:H	2.26	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
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: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: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:C:535:GLY:CA	1:C:553:MET:HE1	2.39	0.51
1:D:378:LEU:CD2	1:D:530:ASP:HB2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLN:HA	4:A:621:HOH:O	2.09	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:C:237:GLU:OE2	1:C:341:HIS:HE1	1.95	0.50
1:B:222:LEU:H	1:B:265:ASN:ND2	2.10	0.50
1:A:466:ASN:H	1:A:466:ASN:HD22	1.60	0.50
1:B:255:LEU:HD22	1:B:380:PHE:CD2	2.47	0.50
1:B:463:VAL:CG2	1:B:468:LEU:HD22	2.42	0.50
1:B:466:ASN:ND2	1:B:466:ASN:H	2.02	0.49
1:B:368:GLU:OE2	1:B:527:LYS:HD2	2.12	0.49
1:C:547:LEU:HG	1:C:551:LYS:HE3	1.94	0.48
1:C:279:GLY:HA2	1:C:313:THR:O	2.14	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:D:463:VAL:HB	1:D:471:MET:HE1	1.96	0.47
1:D:226:VAL:HG11	1:D:252:VAL:HG13	1.96	0.47
1:C:463:VAL:HB	1:C:471:MET:HE1	1.92	0.47
1:C:569:THR:HA	1:C:572:ILE:HD12	1.97	0.47
1:B:331:LEU:HD23	1:B:331:LEU:C	2.36	0.47
1:D:255:LEU:HD21	1:D:380:PHE:CB	2.44	0.47
1:D:463:VAL:HB	1:D:471:MET:HE3	1.94	0.47
1:A:466:ASN:ND2	1:A:466:ASN:H	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:HE3	1:A:247:LYS:HB3	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: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: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: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:B:273:ALA:HB3	1:B:277:PHE:CZ	2.51	0.45
1:D:533:THR:HG22	1:D:553:MET:HE2	1.97	0.45
1:D:238:ARG:HH11	1:D:238:ARG:HG2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:LYS:HE2	1:C:431:ASP:OD2	2.17	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:453:THR:C	1:B:455:GLY:H	2.19	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:D:383:THR:HG23	1:D:553:MET:HE3	1.99	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:HE3	1:D:502:LYS:HB3	1.78	0.43
1:A:519:TYR:CD2	1:A:519:TYR:C	2.91	0.43
1:C:553:MET:HE2	1:C:563:TYR:HE1	1.83	0.43
1:C:378:LEU:HG	1:C:530:ASP:HB2	2.00	0.42
1:A:463:VAL:HB	1:A:471:MET:HE3	1.98	0.42
1:C:553:MET:HE2	1:C:563:TYR:CE1	2.54	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:C:303:ASP:OD2	1:C:305:HIS:HD2	2.02	0.42
1:A:303:ASP:OD2	1:A:305:HIS:CD2	2.72	0.42
1:D:388:THR:OG1	1:D:439:GLY:HA2	2.18	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
1:A:255:LEU:HG	1:A:259:ILE:CD1	2.50	0.41
1:C:361:MET:CG	1:C:519:TYR:CZ	3.03	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:C:273:ALA:HB3	1:C:277:PHE:CZ	2.56	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:A:535:GLY:HA2	1:A:553:MET:HE1	2.01	0.41
1:A:488:ARG:HD3	1:A:490:TYR:OH	2.20	0.41
1:C:331:LEU:C	1:C:331:LEU:HD23	2.41	0.41
1:B:466:ASN:ND2	1:B:466:ASN:N	2.65	0.41
1:D:227:LEU:CD2	1:D:270:VAL:HB	2.50	0.41
1:C:233:SER:OG	1:C:384:ASP:OD2	2.39	0.41
1:D:465:GLN:HB3	1:D:465:GLN:HE21	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
1:B:461:TYR:CE2	1:B:471:MET:HE1	2.57	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%)	46 41
1	B	359/370 (97%)	346 (96%)	12 (3%)	1 (0%)	46 41
1	C	358/370 (97%)	343 (96%)	12 (3%)	3 (1%)	24 15
1	D	355/370 (96%)	339 (96%)	16 (4%)	0	100 100
All	All	1431/1480 (97%)	1376 (96%)	50 (4%)	5 (0%)	46 41

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 (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	315/325 (97%)	301 (96%)	14 (4%)	35 30
1	B	315/325 (97%)	308 (98%)	7 (2%)	60 62
1	C	315/325 (97%)	300 (95%)	15 (5%)	31 26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	312/325 (96%)	296 (95%)	16 (5%)	29 23
All	All	1257/1300 (97%)	1205 (96%)	52 (4%)	37 32

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	254	LYS
1	A	263	LYS
1	A	301	SER
1	A	355	PHE
1	A	456	THR
1	A	457	THR
1	A	463	VAL
1	A	466	ASN
1	A	468	LEU
1	A	469	SER
1	A	525	ARG
1	A	536	ILE
1	A	559	LYS
1	B	355	PHE
1	B	375	ARG
1	B	426	ILE
1	B	463	VAL
1	B	466	ASN
1	B	468	LEU
1	B	559	LYS
1	C	222	LEU
1	C	258	LYS
1	C	263	LYS
1	C	298	ASP
1	C	355	PHE
1	C	376	LYS
1	C	433	GLN
1	C	456	THR
1	C	463	VAL
1	C	465	GLN
1	C	466	ASN
1	C	469	SER
1	C	498	PRO
1	C	559	LYS
1	C	570	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	238	ARG
1	D	254	LYS
1	D	298	ASP
1	D	355	PHE
1	D	375	ARG
1	D	426	ILE
1	D	435	VAL
1	D	453	THR
1	D	456	THR
1	D	463	VAL
1	D	465	GLN
1	D	466	ASN
1	D	525	ARG
1	D	530	ASP
1	D	536	ILE
1	D	572	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	265	ASN
1	A	305	HIS
1	A	341	HIS
1	A	465	GLN
1	A	466	ASN
1	A	508	GLN
1	A	562	ASN
1	B	230	ASN
1	B	265	ASN
1	B	305	HIS
1	B	341	HIS
1	B	466	ASN
1	B	508	GLN
1	B	562	ASN
1	C	265	ASN
1	C	305	HIS
1	C	341	HIS
1	C	422	GLN
1	C	465	GLN
1	C	466	ASN
1	C	467	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	508	GLN
1	D	265	ASN
1	D	305	HIS
1	D	320	ASN
1	D	341	HIS
1	D	465	GLN
1	D	466	ASN
1	D	473	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 carbohydrates 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	A	702	2	1,3,3	2.79	1 (100%)	0,3,3	0.00	-
3	ACT	B	702	2	1,3,3	3.33	1 (100%)	0,3,3	0.00	-
3	ACT	C	702	2	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
3	ACT	D	702	2	1,3,3	2.10	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
3	ACT	A	702	2	-	0/0/0/0	0/0/0/0
3	ACT	B	702	2	-	0/0/0/0	0/0/0/0
3	ACT	C	702	2	-	0/0/0/0	0/0/0/0
3	ACT	D	702	2	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	ACT	CH3-C	2.10	1.51	1.48
3	C	702	ACT	CH3-C	2.40	1.52	1.48
3	A	702	ACT	CH3-C	2.79	1.52	1.48
3	B	702	ACT	CH3-C	3.33	1.53	1.48

There are no bond angle outliers.

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

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	361/370 (97%)	-0.28	2 (0%)	90	90	12, 22, 40, 54	0
1	B	361/370 (97%)	-0.27	2 (0%)	90	90	12, 23, 43, 63	0
1	C	360/370 (97%)	-0.24	7 (1%)	70	70	12, 21, 44, 52	0
1	D	357/370 (96%)	-0.22	6 (1%)	73	73	12, 24, 47, 70	0
All	All	1439/1480 (97%)	-0.25	17 (1%)	81	81	12, 22, 43, 70	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	579	TYR	3.6
1	D	570	ASN	3.3
1	A	465	GLN	2.8
1	D	573	TYR	2.8
1	D	574	ASP	2.7
1	D	571	CYS	2.6
1	C	569	THR	2.6
1	C	574	ASP	2.5
1	C	220	GLN	2.4
1	B	580	PHE	2.3
1	B	577	ASN	2.3
1	C	570	ASN	2.3
1	C	454	GLY	2.3
1	D	465	GLN	2.3
1	A	240	ASN	2.2
1	D	240	ASN	2.0
1	C	567	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ACT	C	702	4/4	0.97	0.13	1.51	16,17,17,17	0
3	ACT	B	702	4/4	0.96	0.12	1.00	16,16,16,18	0
3	ACT	D	702	4/4	0.94	0.11	0.21	21,22,22,22	0
3	ACT	A	702	4/4	0.96	0.09	-0.76	15,16,17,17	0
2	MG	D	701	1/1	0.96	0.05	-2.07	22,22,22,22	0
2	MG	C	701	1/1	0.97	0.05	-2.18	18,18,18,18	0
2	MG	B	701	1/1	0.99	0.06	-2.19	20,20,20,20	0
2	MG	A	701	1/1	0.96	0.04	-3.88	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.