



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:44 PM GMT

PDB ID : 1UZJ  
Title : INTEGRIN BINDING CBEGF22-TB4-CBEGF33 FRAGMENT OF HUMAN FIBRILLIN-1, HOLO FORM.  
Authors : Lee, S.S.J.; Knott, V.; Harlos, K.; Handford, P.A.; Stuart, D.I.  
Deposited on : 2004-03-12  
Resolution : 2.25 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

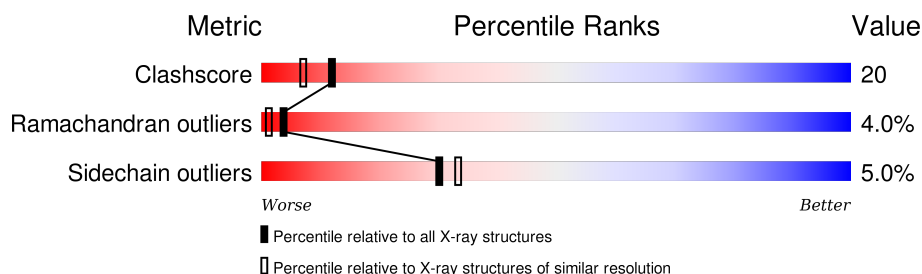
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	 67% 27% 6% •
1	B	162	 73% 23% •
1	C	162	 62% 31% 6%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3806 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 FIBRILLIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1195	725	202	247	21			
1	B	162	Total	C	N	O	S	0	0	0
			1195	725	202	247	21			
1	C	162	Total	C	N	O	S	0	0	0
			1195	725	202	247	21			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

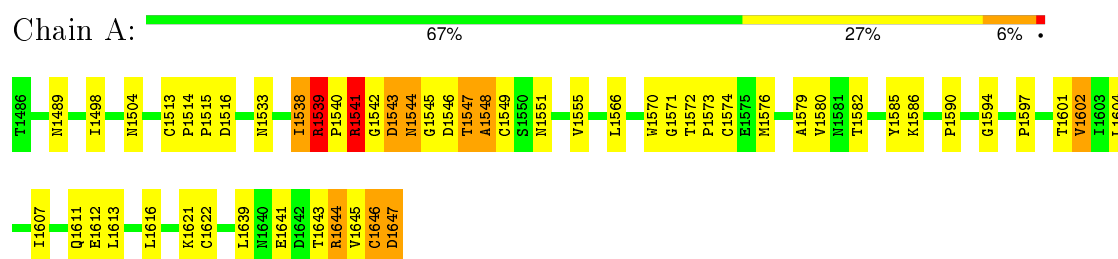
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	79	Total	O	0	0
			79	79		
3	C	55	Total	O	0	0
			55	55		

### 3 Residue-property plots

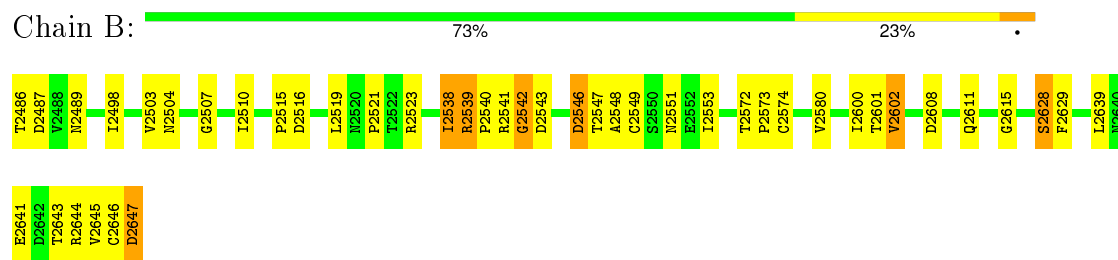
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

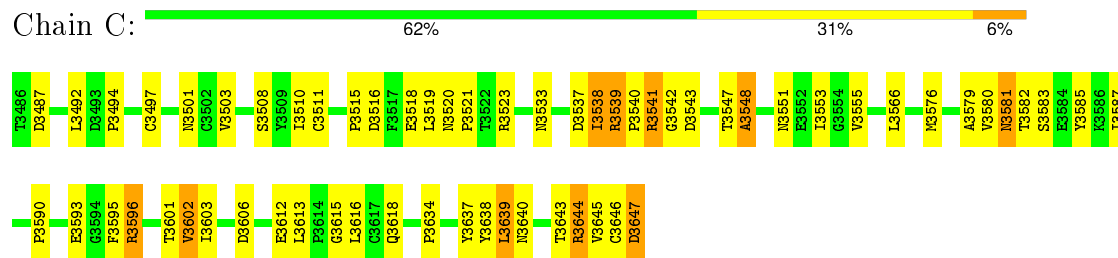
#### • Molecule 1: FIBRILLIN-1



#### • Molecule 1: FIBRILLIN-1



#### • Molecule 1: FIBRILLIN-1



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.10 Å   105.60 Å   65.00 Å 90.00°   104.20°   90.00°	Depositor
Resolution (Å)	30.00 – 2.25	Depositor
% Data completeness (in resolution range)	96.2 (30.00-2.25)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.247 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0/1218	0.73	0/1659
1	B	0.48	0/1218	0.75	0/1659
1	C	0.40	0/1218	0.69	0/1659
All	All	0.47	0/3654	0.73	0/4977

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

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	1195	0	1100	45	0
1	B	1195	0	1100	39	0
1	C	1195	0	1100	56	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	81	0	0	4	0
3	B	79	0	0	4	0
3	C	55	0	0	4	0
All	All	3806	0	3300	138	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 20.

All (138) 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:1538:ILE:HG23	1:A:1539:ARG:H	1.37	0.88
1:C:3497:CYS:HB3	3:C:2018:HOH:O	1.78	0.83
1:A:1548:ALA:HB3	1:A:1574:CYS:SG	2.19	0.83
1:C:3540:PRO:HD2	1:C:3548:ALA:HB1	1.59	0.81
1:C:3511:CYS:HB3	3:C:2018:HOH:O	1.81	0.79
1:C:3618:GLN:HG3	1:C:3645:VAL:HG22	1.67	0.77
1:A:1611:GLN:NE2	1:B:2641:GLU:HB3	2.00	0.77
1:A:1538:ILE:HD13	1:A:1549:CYS:SG	2.25	0.76
1:C:3541:ARG:H	1:C:3541:ARG:HD3	1.50	0.76
1:C:3539:ARG:HD3	1:C:3540:PRO:HD3	1.68	0.74
1:A:1641:GLU:HG2	3:A:2076:HOH:O	1.87	0.74
1:B:2503:VAL:HB	1:B:2510:ILE:HG12	1.69	0.74
1:A:1572:THR:HA	1:A:1573:PRO:C	2.08	0.74
1:B:2538:ILE:HA	3:B:2043:HOH:O	1.87	0.73
1:C:3596:ARG:O	1:C:3596:ARG:HD2	1.89	0.72
1:A:1541:ARG:H	1:A:1541:ARG:HD2	1.53	0.71
1:A:1646:CYS:O	1:A:1647:ASP:HB2	1.91	0.71
1:C:3542:GLY:O	1:C:3547:THR:HA	1.90	0.70
1:B:2498:ILE:HD12	1:B:2602:VAL:HG12	1.73	0.69
1:B:2503:VAL:HB	1:B:2510:ILE:CG1	2.24	0.67
1:B:2519:LEU:HD23	1:B:2523:ARG:HG2	1.78	0.66
1:C:3538:ILE:HA	1:C:3548:ALA:O	1.96	0.65
1:A:1539:ARG:HD2	1:A:1540:PRO:HD2	1.77	0.65
1:B:2538:ILE:HD13	1:B:2549:CYS:SG	2.36	0.65
1:A:1590:PRO:HA	3:A:2047:HOH:O	1.96	0.65
1:B:2601:THR:O	1:B:2602:VAL:HB	1.98	0.64
1:C:3580:VAL:HG12	1:C:3585:TYR:CE2	2.33	0.63
1:C:3615:GLY:HA2	1:C:3618:GLN:NE2	2.15	0.62
1:C:3515:PRO:O	1:C:3516:ASP:HB2	2.00	0.62
1:A:1541:ARG:HD2	1:A:1541:ARG:N	2.14	0.61
1:B:2602:VAL:O	1:B:2602:VAL:HG12	2.00	0.60
1:C:3587:ILE:O	1:C:3590:PRO:HD3	2.01	0.60
1:B:2538:ILE:HD12	3:B:2043:HOH:O	2.01	0.60
1:A:1590:PRO:HG2	1:A:1604:LEU:HD21	1.83	0.59
1:C:3618:GLN:HB2	1:C:3645:VAL:HA	1.84	0.58
1:C:3646:CYS:O	1:C:3647:ASP:HB2	2.03	0.58
1:C:3510:ILE:HD12	1:C:3510:ILE:C	2.25	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3538:ILE:HD13	1:C:3576:MET:HG3	1.87	0.56
1:A:1538:ILE:HG23	1:A:1539:ARG:N	2.16	0.56
1:C:3580:VAL:O	1:C:3580:VAL:HG23	2.05	0.56
1:A:1566:LEU:HD12	1:A:1616:LEU:HD13	1.88	0.56
1:C:3643:THR:O	1:C:3644:ARG:HB2	2.06	0.55
1:A:1571:GLY:O	1:A:1574:CYS:HA	2.06	0.55
1:A:1542:GLY:O	1:A:1543:ASP:HB2	2.05	0.55
1:B:2643:THR:O	1:B:2644:ARG:HB2	2.06	0.55
1:B:2521:PRO:HG2	1:B:2600:ILE:HG23	1.87	0.55
1:C:3593:GLU:HG2	3:C:2045:HOH:O	2.06	0.54
1:B:2541:ARG:HB3	3:B:2003:HOH:O	2.07	0.54
1:C:3640:ASN:OD1	1:C:3643:THR:HG23	2.08	0.54
1:A:1645:VAL:O	1:A:1647:ASP:N	2.41	0.54
1:A:1515:PRO:O	1:A:1516:ASP:HB2	2.07	0.53
1:A:1533:ASN:OD1	1:A:1555:VAL:HA	2.08	0.53
1:A:1621:LYS:HD3	1:A:1622:CYS:N	2.24	0.53
1:C:3583:SER:O	1:C:3587:ILE:HG12	2.08	0.53
1:A:1586:LYS:HD2	3:A:2047:HOH:O	2.07	0.53
1:B:2515:PRO:O	1:B:2516:ASP:HB2	2.09	0.53
1:B:2608:ASP:CG	1:B:2611:GLN:HG3	2.29	0.53
1:A:1611:GLN:NE2	1:B:2641:GLU:CB	2.71	0.52
1:B:2628:SER:OG	1:B:2629:PHE:N	2.43	0.51
1:A:1498:ILE:HB	1:A:1602:VAL:HG11	1.93	0.51
1:A:1643:THR:O	1:A:1644:ARG:HB2	2.10	0.51
1:A:1616:LEU:O	1:A:1644:ARG:HD3	2.11	0.51
1:B:2608:ASP:OD1	1:B:2611:GLN:HG3	2.11	0.51
1:C:3618:GLN:CG	1:C:3645:VAL:HG22	2.39	0.50
1:B:2489:ASN:HA	1:B:2504:ASN:OD1	2.11	0.50
1:A:1572:THR:CA	1:A:1573:PRO:C	2.78	0.50
1:C:3638:TYR:O	1:C:3647:ASP:N	2.45	0.50
1:A:1590:PRO:HG3	1:A:1597:PRO:HG3	1.94	0.50
1:C:3566:LEU:HD12	1:C:3616:LEU:HD13	1.93	0.50
1:C:3612:GLU:O	1:C:3613:LEU:HD23	2.12	0.50
1:A:1579:ALA:HB3	1:A:1582:THR:HG23	1.94	0.50
1:B:2538:ILE:O	1:B:2542:GLY:HA2	2.11	0.49
1:B:2580:VAL:HG22	3:B:2056:HOH:O	2.11	0.49
1:C:3537:ASP:OD1	1:C:3551:ASN:OD1	2.30	0.49
1:C:3538:ILE:HA	1:C:3548:ALA:HB3	1.94	0.49
1:C:3639:LEU:HD23	1:C:3640:ASN:N	2.28	0.49
1:C:3540:PRO:O	1:C:3548:ALA:HB2	2.13	0.48
1:C:3602:VAL:O	1:C:3602:VAL:HG12	2.14	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1572:THR:HA	1:A:1574:CYS:N	2.29	0.48
1:A:1601:THR:C	1:A:1602:VAL:HG23	2.34	0.48
1:B:2543:ASP:HB3	1:B:2546:ASP:O	2.13	0.48
1:B:2519:LEU:HG	1:B:2523:ARG:HA	1.95	0.48
1:A:1580:VAL:HG12	1:A:1585:TYR:CE2	2.49	0.48
1:B:2646:CYS:O	1:B:2647:ASP:HB2	2.12	0.47
1:A:1547:THR:HG23	1:A:1548:ALA:N	2.29	0.47
1:A:1616:LEU:O	1:A:1644:ARG:CD	2.63	0.47
1:C:3595:PHE:CD2	1:C:3606:ASP:HA	2.49	0.47
1:C:3510:ILE:HD12	1:C:3510:ILE:O	2.15	0.47
1:C:3601:THR:OG1	1:C:3603:ILE:HG13	2.15	0.46
1:C:3581:ASN:ND2	3:C:2040:HOH:O	2.47	0.46
1:C:3580:VAL:HG12	1:C:3585:TYR:CZ	2.51	0.46
1:C:3580:VAL:O	1:C:3581:ASN:HB3	2.15	0.46
1:C:3634:PRO:HG2	1:C:3637:TYR:CD2	2.50	0.46
1:C:3515:PRO:O	1:C:3516:ASP:CB	2.64	0.46
1:C:3618:GLN:HG3	1:C:3645:VAL:CG2	2.42	0.46
1:A:1540:PRO:O	1:A:1541:ARG:C	2.55	0.45
1:B:2602:VAL:O	1:B:2602:VAL:CG1	2.64	0.45
1:A:1576:MET:HG2	3:A:2041:HOH:O	2.16	0.45
1:C:3492:LEU:O	1:C:3494:PRO:HD3	2.17	0.45
1:C:3616:LEU:O	1:C:3644:ARG:HD3	2.15	0.45
1:C:3640:ASN:HB3	1:C:3643:THR:OG1	2.16	0.45
1:C:3533:ASN:OD1	1:C:3555:VAL:HA	2.17	0.45
1:B:2572:THR:HA	1:B:2573:PRO:C	2.36	0.45
1:A:1546:ASP:O	1:A:1547:THR:HB	2.16	0.44
1:C:3547:THR:O	1:C:3548:ALA:HB2	2.17	0.44
1:C:3637:TYR:O	1:C:3638:TYR:CD1	2.70	0.44
1:B:2521:PRO:HD2	1:B:2600:ILE:O	2.18	0.44
1:C:3553:ILE:HA	1:C:3615:GLY:HA3	1.99	0.43
1:B:2539:ARG:C	1:B:2541:ARG:N	2.71	0.43
1:B:2628:SER:O	1:B:2629:PHE:HB3	2.18	0.43
1:B:2574:CYS:SG	1:B:2574:CYS:O	2.77	0.43
1:B:2547:THR:HG22	1:B:2548:ALA:N	2.33	0.43
1:B:2539:ARG:HB3	1:B:2540:PRO:HD3	1.99	0.43
1:A:1489:ASN:OD1	1:A:1504:ASN:HB2	2.18	0.43
1:A:1539:ARG:HB3	1:A:1541:ARG:HD3	2.00	0.43
1:C:3520:ASN:HB2	1:C:3521:PRO:HD2	2.00	0.43
1:C:3579:ALA:HB3	1:C:3582:THR:HG23	2.00	0.43
1:C:3539:ARG:N	1:C:3540:PRO:CD	2.82	0.43
1:C:3618:GLN:CB	1:C:3645:VAL:HG22	2.49	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1570:TRP:CG	1:A:1571:GLY:N	2.86	0.42
1:C:3646:CYS:O	1:C:3647:ASP:CB	2.67	0.42
1:B:2539:ARG:C	1:B:2541:ARG:H	2.23	0.42
1:B:2553:ILE:HA	1:B:2615:GLY:HA3	2.01	0.42
1:A:1580:VAL:HA	1:A:1585:TYR:CD2	2.55	0.42
1:B:2542:GLY:HA2	1:B:2547:THR:HG21	2.01	0.42
1:A:1612:GLU:O	1:A:1613:LEU:HD23	2.20	0.41
1:B:2498:ILE:HD12	1:B:2602:VAL:CG1	2.45	0.41
1:B:2645:VAL:O	1:B:2647:ASP:N	2.53	0.41
1:A:1594:GLY:C	1:A:1607:ILE:HD12	2.41	0.41
1:C:3503:VAL:HB	1:C:3510:ILE:HD11	2.03	0.41
1:C:3596:ARG:C	1:C:3596:ARG:CD	2.88	0.41
1:A:1546:ASP:N	1:A:1546:ASP:OD2	2.52	0.41
1:B:2538:ILE:HA	1:B:2538:ILE:HD12	1.95	0.41
1:C:3492:LEU:HD23	1:C:3492:LEU:HA	1.96	0.41
1:A:1544:ASN:HB3	1:A:1545:GLY:H	1.49	0.41
1:B:2487:ASP:OD2	1:B:2507:GLY:N	2.40	0.41
1:C:3519:LEU:CD2	1:C:3523:ARG:HG2	2.51	0.40
1:A:1513:CYS:HA	1:A:1514:PRO:HD3	1.78	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	160/162 (99%)	137 (86%)	16 (10%)	7 (4%)	3	1
1	B	160/162 (99%)	139 (87%)	15 (9%)	6 (4%)	4	1
1	C	160/162 (99%)	135 (84%)	19 (12%)	6 (4%)	4	1
All	All	480/486 (99%)	411 (86%)	50 (10%)	19 (4%)	4	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1602	VAL
1	C	3548	ALA
1	A	1541	ARG
1	A	1543	ASP
1	A	1646	CYS
1	B	2602	VAL
1	C	3538	ILE
1	C	3543	ASP
1	C	3581	ASN
1	B	2542	GLY
1	B	2551	ASN
1	A	1548	ALA
1	A	1538	ILE
1	B	2628	SER
1	C	3508	SER
1	B	2538	ILE
1	B	2539	ARG
1	A	1539	ARG
1	C	3602	VAL

### 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	140/140 (100%)	132 (94%)	8 (6%)	25	26
1	B	140/140 (100%)	136 (97%)	4 (3%)	50	60
1	C	140/140 (100%)	131 (94%)	9 (6%)	22	21
All	All	420/420 (100%)	399 (95%)	21 (5%)	30	33

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1539	ARG
1	A	1541	ARG
1	A	1544	ASN
1	A	1547	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1551	ASN
1	A	1639	LEU
1	A	1644	ARG
1	A	1647	ASP
1	B	2486	THR
1	B	2546	ASP
1	B	2639	LEU
1	B	2647	ASP
1	C	3487	ASP
1	C	3501	ASN
1	C	3518	GLU
1	C	3539	ARG
1	C	3541	ARG
1	C	3596	ARG
1	C	3639	LEU
1	C	3644	ARG
1	C	3647	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1551	ASN
1	A	1618	GLN
1	A	1630	GLN
1	B	2551	ASN
1	B	2630	GLN
1	C	3544	ASN
1	C	3581	ASN
1	C	3630	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.