



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 06:17 AM EDT

PDB ID : 4UM9  
Title : Crystal structure of alpha V beta 6 with peptide  
Authors : Dong, X.; Springer, T.A.  
Deposited on : 2014-05-15  
Resolution : 2.50 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

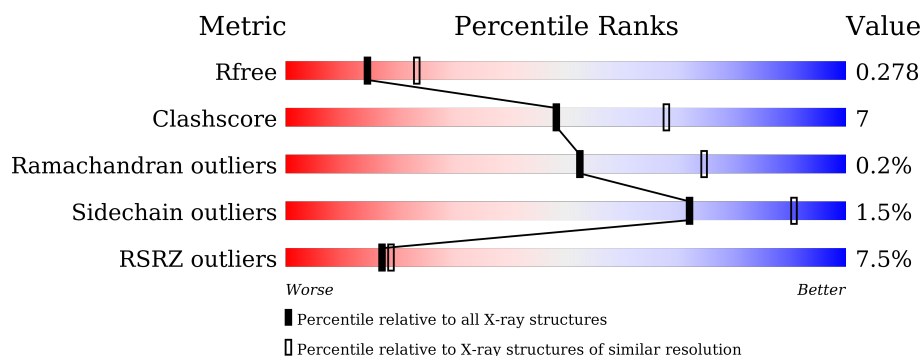
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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.

Mol	Chain	Length	Quality of chain
1	A	604	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	C	604	<div> <div>4%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
2	B	483	<div> <div>11%</div> <div>74%</div> <div>18%</div> <div>7%</div> </div>
3	D	483	<div> <div>13%</div> <div>73%</div> <div>20%</div> <div>6%</div> </div>
4	E	13	<div> <div>69%</div> <div>15%</div> <div>15%</div> </div>
4	F	13	<div> <div>8%</div> <div>85%</div> <div>15%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	NAG	B	3370	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17049 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 INTEGRIN ALPHA-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4601	2917	781	882	21			
1	C	589	Total	C	N	O	S	0	0	0
			4566	2897	774	874	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	596	THR	-	EXPRESSION TAG	UNP P06756
A	597	GLY	-	EXPRESSION TAG	UNP P06756
A	598	GLY	-	EXPRESSION TAG	UNP P06756
A	599	LEU	-	EXPRESSION TAG	UNP P06756
A	600	GLU	-	EXPRESSION TAG	UNP P06756
A	601	VAL	-	EXPRESSION TAG	UNP P06756
A	602	LEU	-	EXPRESSION TAG	UNP P06756
A	603	PHE	-	EXPRESSION TAG	UNP P06756
A	604	GLN	-	EXPRESSION TAG	UNP P06756
A	400	CYS	MET	ENGINEERED MUTATION	UNP P06756
C	596	THR	-	EXPRESSION TAG	UNP P06756
C	597	GLY	-	EXPRESSION TAG	UNP P06756
C	598	GLY	-	EXPRESSION TAG	UNP P06756
C	599	LEU	-	EXPRESSION TAG	UNP P06756
C	600	GLU	-	EXPRESSION TAG	UNP P06756
C	601	VAL	-	EXPRESSION TAG	UNP P06756
C	602	LEU	-	EXPRESSION TAG	UNP P06756
C	603	PHE	-	EXPRESSION TAG	UNP P06756
C	604	GLN	-	EXPRESSION TAG	UNP P06756
C	400	CYS	MET	ENGINEERED MUTATION	UNP P06756

- Molecule 2 is a protein called INTEGRIN BETA-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	448	Total	C	N	O	S	0	0	0
			3433	2155	586	662	30			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	475	SER	-	EXPRESSION TAG	UNP P18564
B	476	ARG	-	EXPRESSION TAG	UNP P18564
B	477	GLY	-	EXPRESSION TAG	UNP P18564
B	478	LEU	-	EXPRESSION TAG	UNP P18564
B	479	GLN	-	EXPRESSION TAG	UNP P18564
B	480	THR	-	EXPRESSION TAG	UNP P18564
B	481	LEU	-	EXPRESSION TAG	UNP P18564
B	482	PHE	-	EXPRESSION TAG	UNP P18564
B	483	GLN	-	EXPRESSION TAG	UNP P18564
B	270	CYS	ILE	CONFLICT	UNP P18564
B	452	ASN	HIS	CONFLICT	UNP P18564

- Molecule 3 is a protein called INTEGRIN BETA-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	455	Total	C	N	O	S	0	0	0
			3485	2185	593	677	30			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	475	SER	-	EXPRESSION TAG	UNP P18564
D	476	ARG	-	EXPRESSION TAG	UNP P18564
D	477	GLY	-	EXPRESSION TAG	UNP P18564
D	478	LEU	-	EXPRESSION TAG	UNP P18564
D	479	GLN	-	EXPRESSION TAG	UNP P18564
D	480	THR	-	EXPRESSION TAG	UNP P18564
D	481	LEU	-	EXPRESSION TAG	UNP P18564
D	482	PHE	-	EXPRESSION TAG	UNP P18564
D	483	GLN	-	EXPRESSION TAG	UNP P18564
D	29	THR	GLN	CONFLICT	UNP P18564
D	270	CYS	ILE	CONFLICT	UNP P18564
D	452	ASN	HIS	CONFLICT	UNP P18564

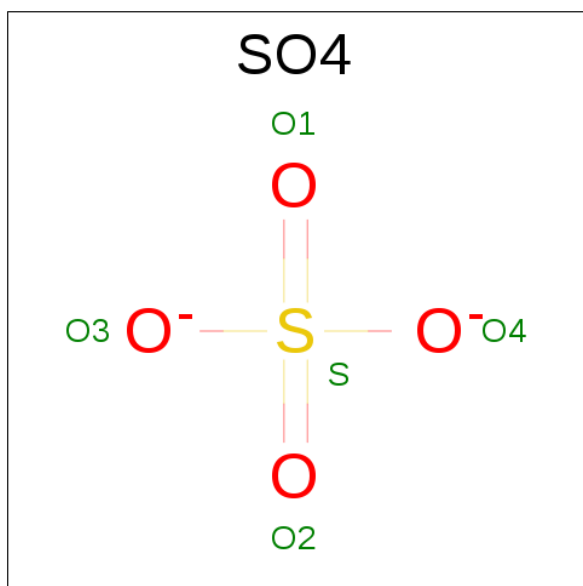
- Molecule 4 is a protein called TRANSFORMING GROWTH FACTOR BETA 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	11	Total	C	N	O	0	0	1
			77	46	19	12			
4	F	13	Total	C	N	O	0	0	2
			89	53	22	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	238	ACE	-	EXPRESSION TAG	UNP Q6TV15
F	238	ACE	-	EXPRESSION TAG	UNP Q6TV15

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Ca 2	0	0
6	A	4	Total 4	Ca 4	0	0
6	D	2	Total 2	Ca 2	0	0
6	C	4	Total 4	Ca 4	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	2	Total 28	C 16	N 2	O 10	0	0
7	A	2	Total 28	C 16	N 2	O 10	0	0
7	A	2	Total 28	C 16	N 2	O 10	0	0
7	A	2	Total 28	C 16	N 2	O 10	0	0
7	C	2	Total 28	C 16	N 2	O 10	0	0
7	C	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	4	Total 50	C 28	N 2	O 20	0	0

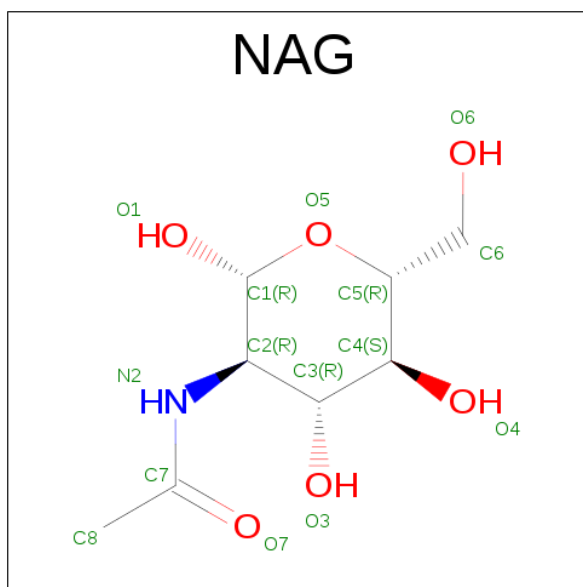
- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	6	Total 72	C 40	N 2	O 30	0	0
9	C	6	Total 72	C 40	N 2	O 30	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Mg 1 1	0	0
10	D	1	Total Mg 1 1	0	0

- Molecule 11 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



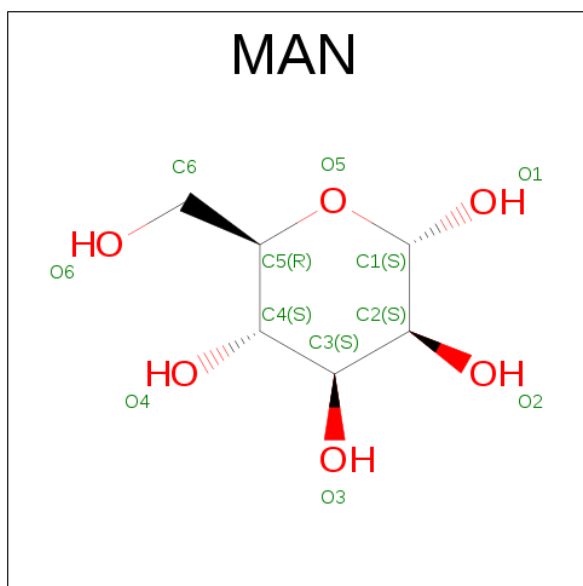
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N O 14 8 1 5	0	0
11	B	1	Total C N O 14 8 1 5	0	0
11	B	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is a polymer of unknown type called SUGAR (3-MER).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			11	6	5		

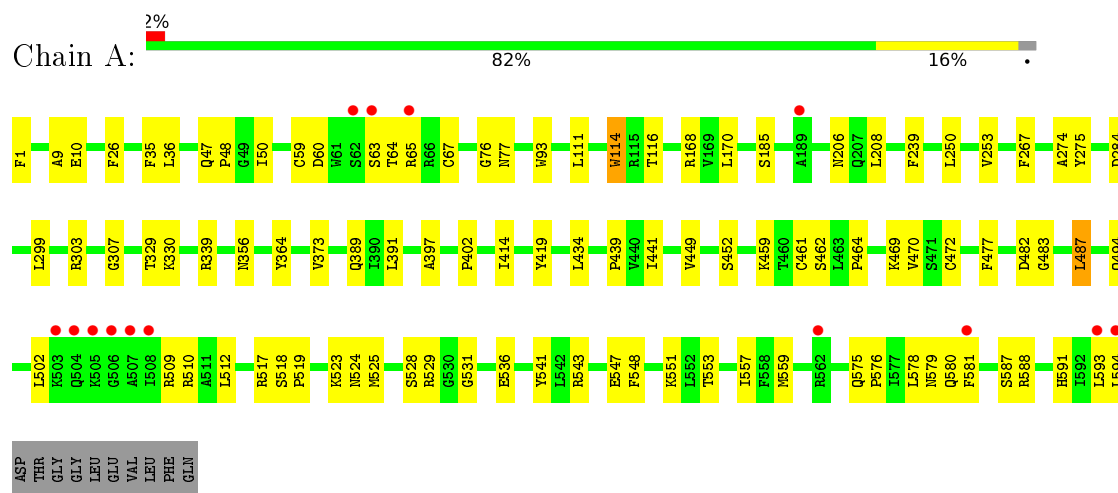
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	89	Total	O	0	0
			89	89		
14	B	64	Total	O	0	0
			64	64		
14	C	53	Total	O	0	0
			53	53		
14	D	22	Total	O	0	0
			22	22		
14	E	2	Total	O	0	0
			2	2		

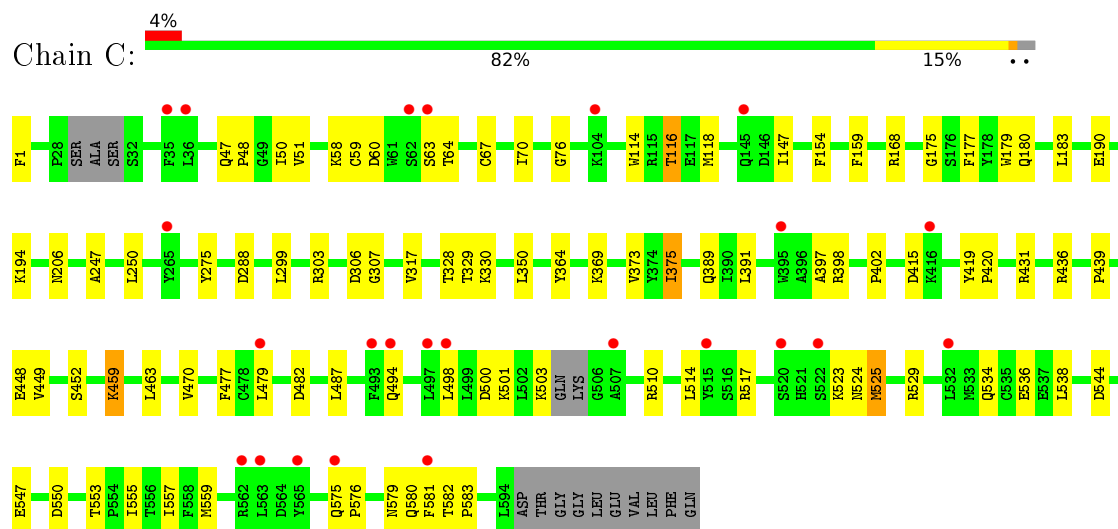
### 3 Residue-property plots

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.

#### • Molecule 1: INTEGRIN ALPHA-V

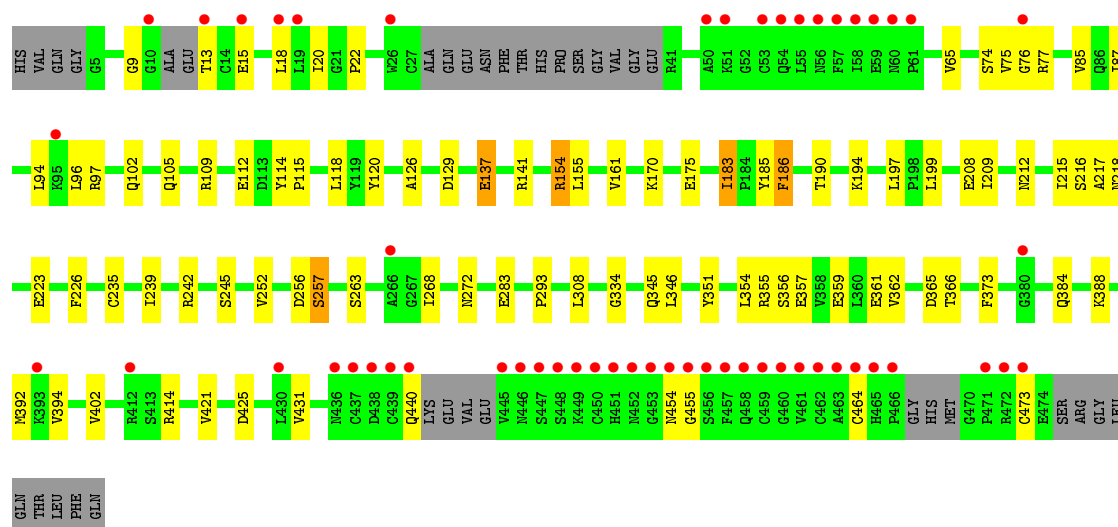


#### • Molecule 1: INTEGRIN ALPHA-V

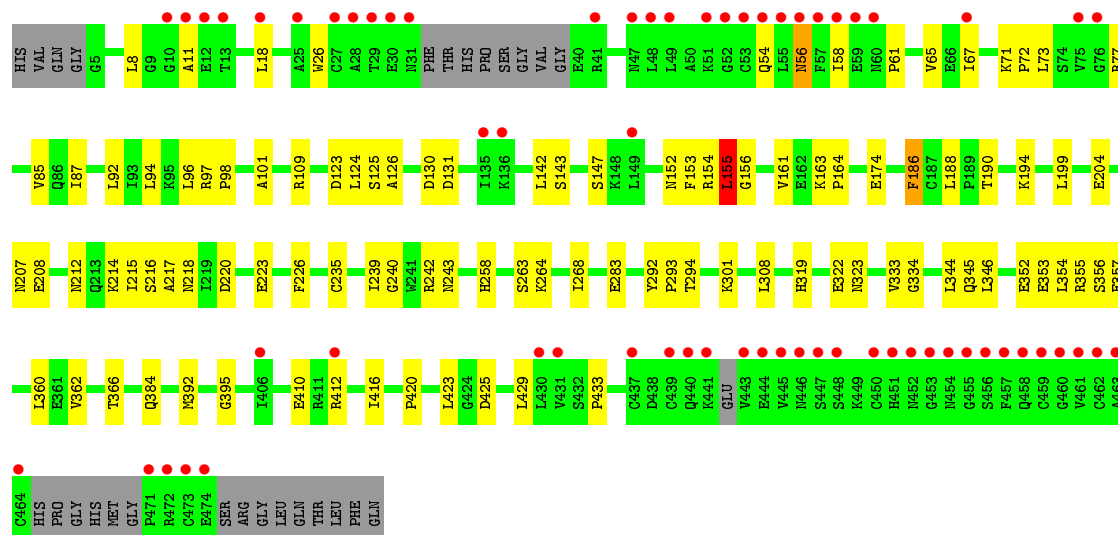
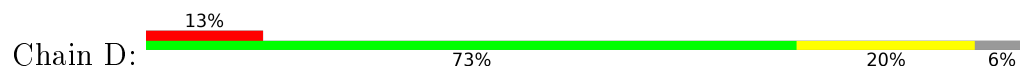


#### • Molecule 2: INTEGRIN BETA-6





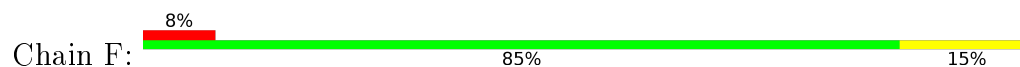
### • Molecule 3: INTEGRIN BETA-6



### • Molecule 4: TRANSFORMING GROWTH FACTOR BETA 3



### • Molecule 4: TRANSFORMING GROWTH FACTOR BETA 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.02Å 168.09Å 101.80Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.50) 94.4 (48.39-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.222 , 0.266 0.232 , 0.278	Depositor DCC
$R_{free}$ test set	1416 reflections (1.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 100046 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, BMA, NAG, ACE, CA, NHH, SO4, MAN

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	0.31	0/4705	0.63	2/6370 (0.0%)
1	C	0.32	0/4668	0.65	2/6318 (0.0%)
2	B	0.30	0/3493	0.61	5/4728 (0.1%)
3	D	0.30	0/3544	0.58	3/4797 (0.1%)
4	E	0.21	0/75	0.32	0/95
4	F	0.20	0/87	0.35	0/112
All	All	0.31	0/16572	0.62	12/22420 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	186	PHE	CB-CG-CD1	-7.15	115.80	120.80
3	D	186	PHE	CB-CG-CD2	6.99	125.69	120.80
1	A	502	LEU	CA-CB-CG	6.14	129.42	115.30
1	C	116	THR	N-CA-C	-5.88	95.13	111.00
2	B	186	PHE	CB-CG-CD1	-5.87	116.69	120.80
2	B	137	GLU	CB-CA-C	-5.70	98.99	110.40
2	B	183	ILE	C-N-CD	-5.52	108.45	120.60
1	C	375	ILE	CG1-CB-CG2	-5.45	99.41	111.40
2	B	186	PHE	CB-CG-CD2	5.38	124.57	120.80
3	D	155	LEU	CA-CB-CG	5.28	127.44	115.30
2	B	154	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	A	487	LEU	CA-CB-CG	5.13	127.11	115.30

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	4601	0	4452	57	1
1	C	4566	0	4414	56	1
2	B	3433	0	3381	63	0
3	D	3485	0	3431	63	0
4	E	77	0	86	2	0
4	F	89	0	94	2	0
5	A	15	0	0	1	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
7	A	112	0	100	0	0
7	C	56	0	50	2	0
8	A	50	0	43	0	0
9	A	72	0	61	0	0
9	C	72	0	61	1	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	42	0	39	0	0
11	C	28	0	26	0	0
11	D	42	0	39	0	0
12	C	39	0	34	2	0
13	C	11	0	10	1	0
14	A	89	0	0	0	0
14	B	64	0	0	2	0
14	C	53	0	0	3	0
14	D	22	0	0	4	0
14	E	2	0	0	0	0
All	All	17049	0	16321	241	1

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 7.

All (241) 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:509:ARG:O	1:A:543:ARG:NH1	2.03	0.91
1:A:494:GLN:NE2	1:A:524:ASN:OD1	2.11	0.84
1:A:10:GLU:H	1:A:65:ARG:HH11	1.35	0.75
3:D:154:ARG:NH2	3:D:240:GLY:O	2.20	0.75
2:B:208:GLU:O	2:B:212:ASN:ND2	2.19	0.74
3:D:152:ASN:N	14:D:4007:HOH:O	2.22	0.72
1:C:494:GLN:NE2	1:C:524:ASN:OD1	2.23	0.72
2:B:170:LYS:HB2	2:B:175:GLU:HG2	1.70	0.71
1:A:487:LEU:HD11	1:A:529:ARG:HD3	1.73	0.70
3:D:71:LYS:HD2	3:D:72:PRO:HD2	1.73	0.69
1:C:397:ALA:HB2	1:C:402:PRO:HD3	1.73	0.69
1:A:10:GLU:H	1:A:65:ARG:NH1	1.90	0.69
1:A:303:ARG:HD2	1:A:307:GLY:O	1.93	0.69
1:C:190:GLU:OE2	1:C:206:ASN:ND2	2.25	0.68
1:C:415:ASP:OD2	14:C:4040:HOH:O	2.12	0.67
3:D:420:PRO:HG2	3:D:423:LEU:HB2	1.76	0.66
2:B:161:VAL:HG21	2:B:216:SER:HB2	1.78	0.66
2:B:186:PHE:HB2	3:D:101:ALA:HB2	1.76	0.65
2:B:15:GLU:OE1	2:B:440:GLN:NE2	2.30	0.65
3:D:125:SER:HB2	4:F:243:ASP:OD1	1.97	0.64
1:A:168:ARG:NH2	1:A:206:ASN:O	2.31	0.63
1:C:58:LYS:HB2	1:C:70:ILE:HD11	1.80	0.63
3:D:263:SER:HB2	3:D:268:ILE:HB	1.79	0.63
2:B:351:TYR:OH	2:B:355:ARG:NH1	2.31	0.62
2:B:129:ASP:OD2	2:B:185:TYR:OH	2.11	0.62
1:C:168:ARG:NH2	1:C:206:ASN:O	2.33	0.62
2:B:18:LEU:HD22	2:B:97:ARG:HH22	1.65	0.62
1:C:503:LYS:NZ	1:C:550:ASP:OD2	2.32	0.61
1:A:63:SER:OG	1:A:64:THR:N	2.32	0.61
1:C:303:ARG:NH1	1:C:307:GLY:O	2.34	0.61
3:D:161:VAL:HG21	3:D:216:SER:HB2	1.82	0.60
1:C:59:CYS:HA	1:C:67:CYS:HA	1.83	0.60
1:C:364:TYR:HB3	1:C:369:LYS:HE2	1.83	0.59
1:C:116:THR:HG22	1:C:118:MET:H	1.67	0.59
3:D:194:LYS:HG2	3:D:283:GLU:HG2	1.83	0.59
1:C:1:PHE:CE1	1:C:580:GLN:HG2	2.38	0.58
1:C:1:PHE:HA	1:C:389:GLN:HB2	1.85	0.58
2:B:455:GLY:HA3	2:B:464:CYS:HA	1.86	0.58
1:C:482:ASP:HA	1:C:529:ARG:HG3	1.87	0.57
1:A:441:ILE:HB	1:A:578:LEU:HD23	1.87	0.57
1:A:548:PHE:O	1:A:551:LYS:NZ	2.28	0.56
3:D:226:PHE:HB3	3:D:293:PRO:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:VAL:HG12	2:B:94:LEU:HD13	1.87	0.56
1:C:436:ARG:HB3	14:C:4040:HOH:O	2.05	0.56
1:C:47:GLN:HB3	1:C:50:ILE:HD12	1.88	0.56
2:B:235:CYS:HB2	2:B:239:ILE:HD13	1.88	0.55
2:B:190:THR:OG1	2:B:217:ALA:O	2.24	0.55
2:B:256:ASP:OD1	2:B:257:SER:N	2.36	0.55
3:D:156:GLY:HA3	3:D:199:LEU:HD12	1.89	0.55
2:B:226:PHE:HB3	2:B:293:PRO:HG2	1.89	0.54
3:D:319:HIS:O	3:D:323:ASN:ND2	2.41	0.54
2:B:96:LEU:HD21	2:B:102:GLN:HB2	1.90	0.54
1:A:47:GLN:HB3	1:A:50:ILE:HD12	1.90	0.53
3:D:362:VAL:HG12	3:D:366:THR:HG21	1.90	0.53
3:D:235:CYS:HB2	3:D:239:ILE:HD13	1.91	0.53
2:B:154:ARG:HH12	2:B:242:ARG:CZ	2.22	0.53
2:B:359:GLU:HB3	2:B:421:VAL:CG2	2.38	0.53
1:C:63:SER:OG	1:C:64:THR:N	2.41	0.53
3:D:56:ASN:N	3:D:56:ASN:OD1	2.42	0.53
3:D:190:THR:OG1	3:D:217:ALA:O	2.27	0.52
12:C:3458:NAG:H61	12:C:3459:NAG:N2	2.25	0.52
3:D:97:ARG:HD2	3:D:98:PRO:HD2	1.92	0.52
2:B:197:LEU:HB2	2:B:209:ILE:HD13	1.92	0.52
3:D:18:LEU:HA	3:D:97:ARG:HH21	1.75	0.52
2:B:263:SER:HB2	2:B:268:ILE:HB	1.91	0.51
2:B:126:ALA:HB1	4:E:247:LEU:HD22	1.92	0.51
1:C:159:PHE:CZ	3:D:264:LYS:HE2	2.46	0.51
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.92	0.51
1:C:498:LEU:HD23	1:C:501:LYS:HD2	1.93	0.51
12:C:3459:NAG:H61	12:C:3460:BMA:O5	2.11	0.50
2:B:215:ILE:H	2:B:215:ILE:HD12	1.76	0.50
1:C:544:ASP:HB3	1:C:547:GLU:HG3	1.94	0.50
3:D:188:LEU:HD12	3:D:214:LYS:HB2	1.93	0.50
3:D:87:ILE:HD12	3:D:420:PRO:HD3	1.93	0.50
1:A:551:LYS:HB3	1:A:594:LEU:HD11	1.92	0.50
2:B:137:GLU:O	2:B:141:ARG:HG3	2.12	0.49
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.95	0.49
2:B:115:PRO:HB2	2:B:245:SER:CB	2.42	0.49
2:B:77:ARG:HB2	2:B:112:GLU:HB2	1.95	0.49
1:A:414:ILE:HG21	1:A:434:LEU:HD21	1.93	0.49
1:C:50:ILE:HD11	1:C:76:GLY:HA2	1.93	0.49
3:D:142:LEU:HA	3:D:344:LEU:HD11	1.94	0.49
3:D:204:GLU:HA	3:D:207:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:126:ALA:HB1	4:F:247:LEU:HD12	1.94	0.49
3:D:208:GLU:O	3:D:212:ASN:ND2	2.40	0.49
1:C:463:LEU:HD21	1:C:517:ARG:HE	1.76	0.49
3:D:322:GLU:CG	3:D:333:VAL:HG21	2.43	0.49
1:A:523:LYS:HG2	1:A:536:GLU:OE1	2.13	0.49
3:D:353:GLU:O	3:D:357:GLU:HG3	2.13	0.48
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.95	0.48
2:B:105:GLN:NE2	14:B:4005:HOH:O	2.45	0.48
1:A:575:GLN:HA	1:A:576:PRO:HD3	1.73	0.48
1:A:114:TRP:CZ2	1:A:116:THR:HA	2.48	0.48
1:A:543:ARG:HD3	1:A:547:GLU:OE1	2.13	0.48
1:C:350:LEU:HA	1:C:420:PRO:HG2	1.96	0.48
1:A:487:LEU:CD1	1:A:529:ARG:HD3	2.43	0.48
3:D:161:VAL:HG21	3:D:216:SER:CB	2.44	0.48
2:B:94:LEU:HG	2:B:96:LEU:HG	1.96	0.48
1:C:579:ASN:OD1	1:C:580:GLN:N	2.47	0.48
3:D:416:ILE:HB	3:D:429:LEU:HB2	1.96	0.48
1:A:472:CYS:HA	1:A:541:TYR:HA	1.96	0.47
1:C:431:ARG:NH2	14:C:4041:HOH:O	2.41	0.47
3:D:73:LEU:HD23	3:D:85:VAL:HG12	1.95	0.47
1:C:523:LYS:HG2	1:C:536:GLU:OE1	2.14	0.47
1:C:525:MET:HE2	1:C:534:GLN:HB3	1.96	0.47
3:D:322:GLU:HG2	3:D:333:VAL:HG21	1.97	0.47
1:A:77:ASN:ND2	5:A:1597:SO4:O2	2.45	0.47
1:A:397:ALA:HB2	1:A:402:PRO:HD3	1.97	0.47
2:B:9:GLY:HA3	2:B:20:ILE:HD13	1.97	0.47
1:C:154:PHE:O	1:C:175:GLY:HA3	2.15	0.47
1:C:250:LEU:HA	1:C:250:LEU:HD12	1.79	0.47
1:A:10:GLU:N	1:A:65:ARG:HH11	2.06	0.47
2:B:13:THR:HG22	2:B:15:GLU:H	1.79	0.47
2:B:115:PRO:HB2	2:B:245:SER:HB3	1.96	0.47
2:B:362:VAL:HG12	2:B:366:THR:HG21	1.97	0.47
2:B:118:LEU:O	2:B:155:LEU:HA	2.15	0.46
3:D:65:VAL:HG12	3:D:94:LEU:HD13	1.97	0.46
1:A:509:ARG:HG2	1:A:519:PRO:HG3	1.98	0.46
2:B:87:ILE:HG22	2:B:425:ASP:HB3	1.98	0.46
3:D:94:LEU:HG	3:D:96:LEU:HG	1.96	0.46
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.97	0.46
1:C:459:LYS:HA	1:C:470:VAL:C	2.36	0.46
3:D:308:LEU:HD13	3:D:354:LEU:HD13	1.98	0.46
2:B:357:GLU:OE1	2:B:388:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:HG22	1:A:330:LYS:H	1.81	0.46
2:B:154:ARG:HH12	2:B:242:ARG:NH2	2.14	0.46
1:C:329:THR:HG22	1:C:330:LYS:H	1.81	0.46
1:A:26:PHE:HB3	1:A:35:PHE:HB2	1.98	0.46
1:C:116:THR:HG23	1:C:147:ILE:HG21	1.97	0.46
3:D:410:GLU:HB2	3:D:433:PRO:HG2	1.98	0.46
2:B:308:LEU:HD13	2:B:354:LEU:HD13	1.98	0.45
1:A:449:VAL:HG21	1:A:557:ILE:HD13	1.98	0.45
1:A:464:PRO:O	1:A:517:ARG:NH2	2.50	0.45
1:C:247:ALA:O	1:C:250:LEU:HB2	2.17	0.45
3:D:264:LYS:HG3	14:D:4018:HOH:O	2.16	0.45
3:D:356:SER:HB2	3:D:392:MET:H	1.79	0.45
3:D:220:ASP:OD2	3:D:258:HIS:NE2	2.43	0.45
2:B:22:PRO:HA	2:B:97:ARG:HH11	1.81	0.45
3:D:174:GLU:H	3:D:174:GLU:CD	2.20	0.45
1:A:482:ASP:HA	1:A:529:ARG:HG3	1.98	0.45
2:B:359:GLU:HG3	2:B:388:LYS:HB2	1.97	0.45
7:C:3585:NAG:H61	7:C:3586:NAG:H82	1.99	0.45
2:B:454:ASN:HB3	2:B:473:CYS:SG	2.57	0.45
1:C:498:LEU:HD23	1:C:501:LYS:CD	2.47	0.45
3:D:87:ILE:HG22	3:D:425:ASP:HB3	1.98	0.45
1:C:449:VAL:HG21	1:C:557:ILE:HD13	1.99	0.45
2:B:197:LEU:HB2	2:B:209:ILE:CD1	2.47	0.44
1:A:587:SER:O	1:A:588:ARG:HD3	2.17	0.44
3:D:186:PHE:HE2	3:D:214:LYS:HZ1	1.64	0.44
3:D:54:GLN:O	3:D:58:ILE:HG13	2.16	0.44
1:C:175:GLY:HA2	1:C:179:TRP:CD1	2.52	0.44
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.85	0.44
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.53	0.44
2:B:120:TYR:CZ	2:B:252:VAL:HG21	2.52	0.44
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.88	0.43
1:A:274:ALA:HA	1:A:299:LEU:HB2	2.00	0.43
1:A:509:ARG:HG2	1:A:519:PRO:CG	2.48	0.43
2:B:414:ARG:HG3	2:B:431:VAL:HB	2.00	0.43
1:C:190:GLU:HG2	1:C:194:LYS:HD3	1.99	0.43
3:D:109:ARG:NH1	3:D:395:GLY:O	2.47	0.43
2:B:154:ARG:HH21	2:B:199:LEU:CD1	2.31	0.43
1:A:579:ASN:OD1	1:A:580:GLN:N	2.51	0.43
2:B:351:TYR:O	2:B:355:ARG:HG2	2.19	0.43
3:D:130:ASP:OD1	3:D:131:ASP:N	2.52	0.43
2:B:359:GLU:HB3	2:B:421:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:143:SER:O	3:D:147:SER:OG	2.27	0.43
3:D:11:ALA:HA	3:D:26:TRP:HZ3	1.83	0.43
9:C:3268:BMA:H62	9:C:3270:MAN:H2	1.75	0.43
1:C:47:GLN:HA	1:C:48:PRO:HD3	1.85	0.43
3:D:301:LYS:HA	3:D:301:LYS:HD3	1.84	0.43
1:A:477:PHE:HB2	1:A:559:MET:SD	2.59	0.43
1:A:339:ARG:HD2	1:A:364:TYR:CE2	2.53	0.43
1:A:529:ARG:C	1:A:531:GLY:H	2.21	0.43
1:A:459:LYS:HA	1:A:470:VAL:C	2.40	0.43
3:D:123:ASP:OD2	3:D:125:SER:OG	2.37	0.43
1:A:253:VAL:HB	1:A:267:PHE:HB2	2.00	0.42
1:A:284:ASP:O	1:A:356:ASN:HB2	2.19	0.42
2:B:114:TYR:HA	2:B:115:PRO:HD3	1.75	0.42
2:B:74:SER:OG	2:B:85:VAL:N	2.46	0.42
1:C:373:VAL:HB	1:C:391:LEU:HB2	2.00	0.42
1:A:170:LEU:HD22	1:A:239:PHE:CD1	2.54	0.42
2:B:161:VAL:HG21	2:B:216:SER:CB	2.47	0.42
2:B:356:SER:O	2:B:392:MET:HG2	2.19	0.42
3:D:352:GLU:HA	3:D:355:ARG:HB2	2.01	0.42
1:A:483:GLY:HA3	1:A:487:LEU:HD21	1.99	0.42
1:A:59:CYS:HA	1:A:67:CYS:HA	2.01	0.42
2:B:183:ILE:HD11	4:E:244:LEU:HD22	2.01	0.42
2:B:362:VAL:HG21	2:B:373:PHE:HZ	1.84	0.42
3:D:18:LEU:HD13	3:D:61:PRO:HG3	2.01	0.42
1:C:487:LEU:HG	1:C:529:ARG:HD3	2.01	0.42
3:D:152:ASN:CB	14:D:4007:HOH:O	2.68	0.42
3:D:163:LYS:HE2	3:D:292:TYR:CE1	2.55	0.42
3:D:360:LEU:HA	3:D:360:LEU:HD23	1.70	0.42
2:B:361:GLU:OE2	2:B:421:VAL:HG22	2.20	0.42
1:C:510:ARG:NH1	1:C:553:THR:O	2.47	0.42
1:A:518:SER:HA	1:A:519:PRO:HD3	1.88	0.42
1:C:477:PHE:HB2	1:C:559:MET:SD	2.60	0.42
1:C:500:ASP:OD1	1:C:503:LYS:HG2	2.20	0.42
1:A:462:SER:HA	1:A:469:LYS:HG2	2.02	0.42
1:C:575:GLN:HA	1:C:576:PRO:HD3	1.79	0.42
3:D:223:GLU:HB2	14:D:4015:HOH:O	2.20	0.42
2:B:76:GLY:O	2:B:77:ARG:HB3	2.19	0.42
1:C:582:THR:HA	1:C:583:PRO:HD3	1.86	0.42
3:D:67:ILE:HA	3:D:92:LEU:HD23	2.02	0.42
1:C:306:ASP:N	1:C:306:ASP:OD1	2.36	0.42
1:C:177:PHE:O	1:C:180:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.89	0.41
1:C:580:GLN:O	1:C:581:PHE:HB3	2.20	0.41
3:D:154:ARG:HH12	3:D:242:ARG:CZ	2.33	0.41
1:A:50:ILE:HD11	1:A:76:GLY:HA2	2.02	0.41
2:B:365:ASP:HB3	2:B:414:ARG:HB2	2.01	0.41
1:C:500:ASP:HB2	1:C:555:ILE:HG23	2.01	0.41
2:B:373:PHE:CD2	2:B:402:VAL:HG22	2.56	0.41
1:C:317:VAL:O	1:C:328:THR:HA	2.21	0.41
7:C:3260:NAG:H61	7:C:3261:NAG:C7	2.49	0.41
1:A:93:TRP:CD1	1:A:111:LEU:HD12	2.56	0.41
1:A:461:CYS:N	1:A:472:CYS:SG	2.92	0.41
1:A:510:ARG:NH1	1:A:553:THR:O	2.48	0.41
2:B:355:ARG:HH21	2:B:394:VAL:HG11	1.86	0.41
2:B:308:LEU:HD21	2:B:421:VAL:HG12	2.02	0.41
1:C:299:LEU:HD22	3:D:294:THR:HG21	2.03	0.41
3:D:345:GLN:OE1	3:D:345:GLN:N	2.39	0.41
2:B:223:GLU:HB2	14:B:4036:HOH:O	2.20	0.41
2:B:334:GLY:HA3	2:B:346:LEU:HD22	2.02	0.41
3:D:124:LEU:HD23	3:D:124:LEU:HA	1.94	0.41
3:D:153:PHE:CE2	3:D:155:LEU:HG	2.56	0.41
1:A:580:GLN:HG3	1:A:581:PHE:N	2.36	0.41
1:C:288:ASP:OD1	1:C:288:ASP:N	2.54	0.41
2:B:154:ARG:NH2	2:B:242:ARG:HG2	2.36	0.41
3:D:334:GLY:HA3	3:D:346:LEU:HD22	2.03	0.41
1:A:185:SER:HB3	1:A:208:LEU:HB2	2.02	0.41
1:C:419:TYR:CE1	1:C:439:PRO:HA	2.56	0.41
2:B:75:VAL:HB	2:B:109:ARG:NH1	2.36	0.40
2:B:194:LYS:HG2	2:B:283:GLU:HG2	2.02	0.40
1:C:375:ILE:CD1	1:C:391:LEU:HD13	2.51	0.40
1:C:448:GLU:OE1	13:C:3461:MAN:O3	2.24	0.40
2:B:272:ASN:HD22	2:B:293:PRO:HD3	1.87	0.40
1:C:580:GLN:C	1:C:582:THR:H	2.25	0.40
3:D:163:LYS:HA	3:D:164:PRO:HD3	1.87	0.40
3:D:126:ALA:HA	3:D:215:ILE:CG2	2.51	0.40
2:B:345:GLN:OE1	2:B:345:GLN:N	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:SER:OG	1:C:452:SER:OG[4_555]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	592/604 (98%)	567 (96%)	24 (4%)	1 (0%)	52	75
1	C	583/604 (96%)	564 (97%)	18 (3%)	1 (0%)	52	75
2	B	438/483 (91%)	418 (95%)	20 (5%)	0	100	100
3	D	447/483 (92%)	424 (95%)	21 (5%)	2 (0%)	39	61
4	E	8/13 (62%)	8 (100%)	0	0	100	100
4	F	10/13 (77%)	10 (100%)	0	0	100	100
All	All	2078/2200 (94%)	1991 (96%)	83 (4%)	4 (0%)	52	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	LEU
1	C	459	LYS
3	D	8	LEU
3	D	77	ARG

### 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	487/495 (98%)	480 (99%)	7 (1%)	74	91
1	C	483/495 (98%)	473 (98%)	10 (2%)	61	85
2	B	393/421 (93%)	390 (99%)	3 (1%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	398/421 (94%)	392 (98%)	6 (2%)	72	91
4	E	7/8 (88%)	7 (100%)	0	100	100
4	F	8/8 (100%)	8 (100%)	0	100	100
All	All	1776/1848 (96%)	1750 (98%)	26 (2%)	72	91

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	114	TRP
1	A	275	TYR
1	A	512	LEU
1	A	525	MET
1	A	528	SER
1	A	591	HIS
2	B	218	ASN
2	B	257	SER
2	B	384	GLN
1	C	51	VAL
1	C	60	ASP
1	C	114	TRP
1	C	183	LEU
1	C	275	TYR
1	C	398	ARG
1	C	479	LEU
1	C	514	LEU
1	C	525	MET
1	C	538	LEU
3	D	56	ASN
3	D	155	LEU
3	D	218	ASN
3	D	243	ASN
3	D	384	GLN
3	D	412	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	GLN
1	C	327	GLN

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Mol	Chain	Res	Type
1	C	494	GLN
1	C	534	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 ⓘ

31 carbohydrates 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	$\# Z  > 2$
7	NAG	A	3044	1,7	14,14,15	0.27	0	15,19,21	0.41	0
7	NAG	A	3045	7	14,14,15	0.29	0	15,19,21	0.48	0
8	NAG	A	3260	1,8	14,14,15	0.20	0	15,19,21	0.27	0
8	NAG	A	3261	8	14,14,15	0.17	0	15,19,21	0.34	0
8	BMA	A	3262	8	11,11,12	0.71	0	15,15,17	0.96	0
8	MAN	A	3263	8	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
9	NAG	A	3266	1,9	14,14,15	0.51	0	15,19,21	0.33	0
9	NAG	A	3267	9	14,14,15	0.40	0	15,19,21	0.30	0
9	BMA	A	3268	9	11,11,12	0.88	1 (9%)	15,15,17	0.73	0
9	MAN	A	3269	9	11,11,12	0.73	1 (9%)	15,15,17	0.92	1 (6%)
9	MAN	A	3270	9	11,11,12	0.79	1 (9%)	15,15,17	0.88	1 (6%)
9	MAN	A	3271	9	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
7	NAG	A	3458	1,7	14,14,15	0.70	0	15,19,21	0.32	0
7	NAG	A	3459	7	14,14,15	0.29	0	15,19,21	0.37	0
7	NAG	A	3524	1,7	14,14,15	0.52	0	15,19,21	0.64	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	3525	7	14,14,15	0.31	0	15,19,21	0.31	0
7	NAG	A	3585	1,7	14,14,15	0.33	0	15,19,21	0.31	0
7	NAG	A	3586	7	14,14,15	0.31	0	15,19,21	0.38	0
7	NAG	C	3260	1,7	14,14,15	0.18	0	15,19,21	0.43	0
7	NAG	C	3261	7	14,14,15	0.21	0	15,19,21	0.40	0
9	NAG	C	3266	1,9	14,14,15	0.49	0	15,19,21	0.44	0
9	NAG	C	3267	9	14,14,15	0.25	0	15,19,21	0.31	0
9	BMA	C	3268	9	11,11,12	0.80	1 (9%)	15,15,17	0.79	1 (6%)
9	MAN	C	3269	9	11,11,12	0.68	0	15,15,17	0.93	2 (13%)
9	MAN	C	3270	9	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
9	MAN	C	3271	9	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
12	NAG	C	3458	1,12	14,14,15	0.72	1 (7%)	15,19,21	0.32	0
12	NAG	C	3459	12	14,14,15	0.73	1 (7%)	15,19,21	0.97	1 (6%)
12	BMA	C	3460	12	11,11,12	0.95	1 (9%)	15,15,17	2.63	4 (26%)
7	NAG	C	3585	1,7	14,14,15	0.45	0	15,19,21	0.34	0
7	NAG	C	3586	7	14,14,15	0.44	0	15,19,21	0.44	0

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
7	NAG	A	3044	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	3045	7	-	0/6/23/26	0/1/1/1
8	NAG	A	3260	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	3261	8	-	0/6/23/26	0/1/1/1
8	BMA	A	3262	8	-	0/2/19/22	0/1/1/1
8	MAN	A	3263	8	-	0/2/19/22	0/1/1/1
9	NAG	A	3266	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	3267	9	-	0/6/23/26	0/1/1/1
9	BMA	A	3268	9	-	0/2/19/22	0/1/1/1
9	MAN	A	3269	9	-	0/2/19/22	0/1/1/1
9	MAN	A	3270	9	-	0/2/19/22	0/1/1/1
9	MAN	A	3271	9	-	0/2/19/22	0/1/1/1
7	NAG	A	3458	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	3459	7	-	0/6/23/26	0/1/1/1
7	NAG	A	3524	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	3525	7	-	0/6/23/26	0/1/1/1
7	NAG	A	3585	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	3586	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	3260	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	3261	7	-	0/6/23/26	0/1/1/1
9	NAG	C	3266	1,9	-	0/6/23/26	0/1/1/1
9	NAG	C	3267	9	-	0/6/23/26	0/1/1/1
9	BMA	C	3268	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3269	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3270	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3271	9	-	0/2/19/22	0/1/1/1
12	NAG	C	3458	1,12	-	0/6/23/26	0/1/1/1
12	NAG	C	3459	12	-	0/6/23/26	0/1/1/1
12	BMA	C	3460	12	-	0/2/19/22	0/1/1/1
7	NAG	C	3585	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	3586	7	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	3459	NAG	O5-C1	-2.61	1.39	1.43
9	A	3268	BMA	O5-C1	-2.50	1.39	1.43
12	C	3458	NAG	O5-C1	-2.46	1.39	1.43
9	A	3270	MAN	O5-C1	-2.22	1.40	1.43
9	C	3268	BMA	O5-C1	-2.14	1.40	1.43
9	A	3269	MAN	O5-C1	-2.00	1.40	1.43
12	C	3460	BMA	C1-C2	2.26	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	3460	BMA	C1-C2-C3	-6.36	101.85	109.55
12	C	3460	BMA	C3-C4-C5	-3.20	104.52	110.23
12	C	3459	NAG	O4-C4-C3	-2.94	103.72	110.36
12	C	3460	BMA	O5-C5-C4	-2.61	105.81	110.13
9	C	3270	MAN	O2-C2-C3	-2.43	105.29	110.19
9	A	3269	MAN	O2-C2-C3	-2.22	105.71	110.19
9	A	3270	MAN	O2-C2-C3	-2.20	105.75	110.19
9	C	3269	MAN	O2-C2-C3	-2.18	105.78	110.19
9	A	3271	MAN	O2-C2-C3	-2.18	105.79	110.19
8	A	3263	MAN	O2-C2-C3	-2.15	105.85	110.19
9	C	3268	BMA	O2-C2-C3	-2.15	105.86	110.19
9	C	3271	MAN	O2-C2-C3	-2.10	105.96	110.19
7	A	3524	NAG	C1-O5-C5	2.02	115.11	112.14
9	C	3269	MAN	C1-O5-C5	2.07	115.19	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	3271	MAN	C1-O5-C5	2.27	115.47	112.14
8	A	3263	MAN	C1-O5-C5	2.30	115.52	112.14
9	C	3270	MAN	C1-O5-C5	2.34	115.58	112.14
9	A	3271	MAN	C1-O5-C5	2.46	115.75	112.14
12	C	3460	BMA	O3-C3-C2	5.80	120.63	110.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	3260	NAG	1	0
7	C	3261	NAG	1	0
9	C	3268	BMA	1	0
9	C	3270	MAN	1	0
12	C	3458	NAG	1	0
12	C	3459	NAG	2	0
12	C	3460	BMA	1	0
7	C	3585	NAG	1	0
7	C	3586	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 14 are monoatomic - leaving 15 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	$\# Z  > 2$
5	SO4	A	1595	-	4,4,4	0.25	0	6,6,6	0.10	0
5	SO4	A	1596	-	4,4,4	0.26	0	6,6,6	0.09	0
5	SO4	A	1597	-	4,4,4	0.32	0	6,6,6	0.15	0
5	SO4	B	1475	-	4,4,4	0.28	0	6,6,6	0.08	0
11	NAG	B	3080	2	14,14,15	0.26	0	15,19,21	0.26	0
11	NAG	B	3243	2	14,14,15	0.33	0	15,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	B	3370	2	14,14,15	0.63	1 (7%)	15,19,21	0.51	0
5	SO4	C	1595	-	4,4,4	0.25	0	6,6,6	0.10	0
5	SO4	C	1596	-	4,4,4	0.23	0	6,6,6	0.06	0
11	NAG	C	3044	1	14,14,15	0.18	0	15,19,21	0.28	0
13	MAN	C	3461	-	11,11,12	1.46	3 (27%)	15,15,17	1.82	3 (20%)
11	NAG	C	3524	1	14,14,15	0.43	0	15,19,21	0.35	0
11	NAG	D	3031	3	14,14,15	0.32	0	15,19,21	0.53	0
11	NAG	D	3080	3	14,14,15	0.35	0	15,19,21	0.35	0
11	NAG	D	3243	3	14,14,15	0.42	0	15,19,21	0.43	0

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
5	SO4	A	1595	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1596	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1597	-	-	0/0/0/0	0/0/0/0
5	SO4	B	1475	-	-	0/0/0/0	0/0/0/0
11	NAG	B	3080	2	-	0/6/23/26	0/1/1/1
11	NAG	B	3243	2	-	0/6/23/26	0/1/1/1
11	NAG	B	3370	2	-	0/6/23/26	0/1/1/1
5	SO4	C	1595	-	-	0/0/0/0	0/0/0/0
5	SO4	C	1596	-	-	0/0/0/0	0/0/0/0
11	NAG	C	3044	1	-	0/6/23/26	0/1/1/1
13	MAN	C	3461	-	-	0/2/19/22	0/1/1/1
11	NAG	C	3524	1	-	0/6/23/26	0/1/1/1
11	NAG	D	3031	3	-	0/6/23/26	0/1/1/1
11	NAG	D	3080	3	-	0/6/23/26	0/1/1/1
11	NAG	D	3243	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	3461	MAN	O5-C1	-2.76	1.39	1.43
13	C	3461	MAN	C1-C2	-2.55	1.45	1.52
13	C	3461	MAN	O5-C5	2.01	1.47	1.43
11	B	3370	NAG	C1-C2	2.17	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
13	C	3461	MAN	C1-C2-C3	-4.74	103.81	109.55
13	C	3461	MAN	O2-C2-C3	-3.09	103.95	110.19
13	C	3461	MAN	O5-C1-C2	3.02	115.73	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1597	SO4	1	0
13	C	3461	MAN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	594/604 (98%)	0.19	14 (2%) 62 66	34, 60, 103, 176	0
1	C	589/604 (97%)	0.29	24 (4%) 41 46	41, 71, 110, 204	0
2	B	448/483 (92%)	0.65	54 (12%) 6 5	25, 61, 148, 228	0
3	D	455/483 (94%)	0.82	64 (14%) 4 3	29, 66, 175, 227	0
4	E	10/13 (76%)	0.55	0 100 100	57, 61, 107, 111	0
4	F	11/13 (84%)	0.50	1 (9%) 11 12	53, 67, 103, 157	0
All	All	2107/2200 (95%)	0.46	157 (7%) 17 19	25, 65, 141, 228	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	473	CYS	13.2
3	D	452	ASN	11.0
3	D	458	GLN	9.1
2	B	462	CYS	8.6
3	D	448	SER	8.3
3	D	457	PHE	8.0
3	D	443	VAL	7.7
2	B	449	LYS	7.7
3	D	52	GLY	7.2
3	D	456	SER	7.2
2	B	58	ILE	7.2
3	D	464	CYS	7.1
2	B	445	VAL	7.1
2	B	50	ALA	7.0
3	D	454	ASN	6.9
3	D	12	GLU	6.9
2	B	464	CYS	6.6
3	D	461	VAL	6.6
2	B	453	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
3	D	462	CYS	6.3
2	B	457	PHE	6.3
2	B	57	PHE	6.2
2	B	450	CYS	6.2
3	D	455	GLY	6.1
2	B	448	SER	6.0
2	B	471	PRO	6.0
2	B	55	LEU	6.0
3	D	445	VAL	6.0
2	B	18	LEU	6.0
2	B	466	PRO	5.8
3	D	28	ALA	5.6
2	B	452	ASN	5.6
3	D	451	HIS	5.5
3	D	11	ALA	5.5
3	D	474	GLU	5.5
2	B	380	GLY	5.5
2	B	456	SER	5.4
3	D	450	CYS	5.4
3	D	54	GLN	5.4
2	B	54	GLN	5.1
3	D	444	GLU	5.1
2	B	465	HIS	4.9
3	D	459	CYS	4.8
3	D	440	GLN	4.8
3	D	30	GLU	4.8
1	C	565	TYR	4.7
3	D	55	LEU	4.7
3	D	60	ASN	4.7
1	C	581	PHE	4.7
1	A	505	LYS	4.6
3	D	441	LYS	4.6
2	B	472	ARG	4.6
2	B	455	GLY	4.5
3	D	58	ILE	4.4
3	D	446	ASN	4.4
3	D	57	PHE	4.4
3	D	75	VAL	4.4
1	C	265	TYR	4.4
2	B	26	TRP	4.3
2	B	451	HIS	4.3
2	B	53	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	439	CYS	4.2
2	B	473	CYS	4.2
3	D	453	GLY	4.1
3	D	437	CYS	4.0
1	C	507	ALA	3.9
3	D	10	GLY	3.8
1	A	506	GLY	3.7
3	D	51	LYS	3.7
3	D	76	GLY	3.7
3	D	472	ARG	3.7
3	D	27	CYS	3.7
3	D	49	LEU	3.7
2	B	461	VAL	3.7
3	D	41	ARG	3.6
3	D	430	LEU	3.6
1	A	503	LYS	3.6
1	C	532	LEU	3.6
3	D	59	GLU	3.5
1	C	62	SER	3.5
2	B	76	GLY	3.4
2	B	459	CYS	3.4
2	B	430	LEU	3.4
3	D	13	THR	3.4
1	C	515	TYR	3.3
3	D	56	ASN	3.3
1	A	507	ALA	3.3
2	B	447	SER	3.3
3	D	53	CYS	3.2
3	D	29	THR	3.2
3	D	460	GLY	3.2
1	A	504	GLN	3.2
2	B	458	GLN	3.2
2	B	437	CYS	3.1
2	B	10	GLY	3.1
2	B	438	ASP	3.0
2	B	56	ASN	3.0
2	B	51	LYS	3.0
3	D	47	ASN	3.0
4	F	239	HIS	3.0
1	A	594	LEU	3.0
1	C	497	LEU	2.9
1	A	63	SER	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	D	136	LYS	2.9
2	B	454	ASN	2.8
1	C	63	SER	2.8
2	B	440	GLN	2.7
2	B	446	ASN	2.7
1	A	65	ARG	2.7
2	B	439	CYS	2.7
2	B	460	GLY	2.7
3	D	48	LEU	2.7
3	D	463	ALA	2.7
2	B	15	GLU	2.6
1	C	522	SER	2.6
1	C	563	LEU	2.6
3	D	25	ALA	2.6
3	D	412	ARG	2.6
1	C	520	SER	2.6
3	D	447	SER	2.6
1	C	498	LEU	2.6
3	D	406	ILE	2.6
1	A	593	LEU	2.6
3	D	471	PRO	2.6
1	A	62	SER	2.6
1	C	395	TRP	2.5
1	C	494	GLN	2.5
2	B	13	THR	2.5
3	D	149	LEU	2.5
1	A	581	PHE	2.5
2	B	60	ASN	2.5
1	C	479	LEU	2.4
1	C	104	LYS	2.4
3	D	31	ASN	2.4
1	A	562	ARG	2.4
1	C	36	LEU	2.4
3	D	18	LEU	2.4
1	A	508	ILE	2.4
2	B	463	ALA	2.3
1	C	575	GLN	2.3
3	D	67	ILE	2.3
2	B	19	LEU	2.3
1	C	416	LYS	2.3
1	A	189	ALA	2.3
2	B	266	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	436	ASN	2.2
2	B	59	GLU	2.2
2	B	412	ARG	2.2
1	C	35	PHE	2.2
1	C	145	GLN	2.2
3	D	431	VAL	2.1
1	C	493	PHE	2.1
2	B	95	LYS	2.1
2	B	61	PRO	2.1
1	C	562	ARG	2.1
3	D	135	ILE	2.0
2	B	393	LYS	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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
12	NAG	C	3459	14/15	0.81	0.19	1.26	106,123,142,150	0
7	NAG	A	3459	14/15	0.82	0.18	1.14	94,125,134,134	0
7	NAG	C	3260	14/15	0.94	0.20	0.77	68,90,100,117	0
7	NAG	A	3458	14/15	0.93	0.16	0.09	67,82,97,103	0
9	NAG	C	3266	14/15	0.97	0.12	-0.76	41,55,65,71	0
7	NAG	A	3044	14/15	0.96	0.11	-0.87	45,54,69,72	0
7	NAG	A	3585	14/15	0.88	0.14	-0.99	80,106,126,149	0
12	NAG	C	3458	14/15	0.94	0.09	-1.04	45,78,89,102	0
9	NAG	A	3266	14/15	0.96	0.13	-1.17	42,49,60,64	0
8	NAG	A	3260	14/15	0.97	0.12	-1.28	46,63,72,79	0
7	NAG	C	3585	14/15	0.90	0.16	-1.58	91,107,140,155	0
7	NAG	A	3045	14/15	0.82	0.30	-	110,137,151,156	0
7	NAG	A	3525	14/15	0.77	0.32	-	133,157,165,169	0
7	NAG	A	3586	14/15	0.81	0.32	-	166,175,183,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	C	3586	14/15	0.58	0.38	-	174,184,193,200	0
8	NAG	A	3261	14/15	0.87	0.21	-	76,98,120,144	0
9	MAN	C	3270	11/12	0.87	0.28	-	149,154,169,176	0
8	BMA	A	3262	11/12	0.58	0.28	-	142,152,156,157	0
9	MAN	A	3271	11/12	0.79	0.40	-	153,161,166,166	0
8	MAN	A	3263	11/12	0.86	0.24	-	129,146,154,158	0
9	MAN	C	3271	11/12	0.65	0.40	-	155,163,173,177	0
12	BMA	C	3460	11/12	0.71	0.21	-	113,119,152,154	0
7	NAG	C	3261	14/15	0.79	0.27	-	76,126,134,141	0
9	NAG	A	3267	14/15	0.95	0.13	-	47,80,87,98	0
9	MAN	C	3269	11/12	0.82	0.41	-	120,148,159,168	0
9	MAN	A	3270	11/12	0.85	0.27	-	159,163,172,181	0
9	BMA	C	3268	11/12	0.92	0.11	-	55,96,131,138	0
9	MAN	A	3269	11/12	0.84	0.39	-	100,135,158,161	0
9	NAG	C	3267	14/15	0.96	0.12	-	39,65,89,97	0
7	NAG	A	3524	14/15	0.81	0.27	-	119,129,160,162	0
9	BMA	A	3268	11/12	0.85	0.16	-	107,119,144,153	0

## 6.4 Ligands ⓘ

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
11	NAG	B	3370	14/15	0.65	0.40	4.14	118,145,153,162	0
5	SO4	A	1596	5/5	0.78	0.19	1.73	198,205,206,226	0
6	CA	D	2002	1/1	0.78	0.19	0.55	140,140,140,140	0
5	SO4	A	1597	5/5	0.98	0.16	0.42	82,89,99,101	0
6	CA	A	2002	1/1	0.97	0.14	0.23	58,58,58,58	0
6	CA	A	2003	1/1	0.97	0.13	-0.56	53,53,53,53	0
6	CA	C	2002	1/1	0.96	0.12	-0.62	68,68,68,68	0
6	CA	D	2003	1/1	0.97	0.17	-0.63	49,49,49,49	0
11	NAG	C	3044	14/15	0.93	0.11	-0.96	55,65,78,85	0
6	CA	B	2002	1/1	0.99	0.18	-0.98	47,47,47,47	0
6	CA	A	2001	1/1	0.94	0.13	-1.19	67,67,67,67	0
6	CA	A	2004	1/1	0.98	0.10	-1.67	45,45,45,45	0
6	CA	C	2004	1/1	0.95	0.08	-1.68	62,62,62,62	0
5	SO4	C	1595	5/5	0.97	0.11	-1.94	66,69,86,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CA	C	2001	1/1	0.63	0.08	-2.09	73,73,73,73	0
6	CA	C	2003	1/1	0.94	0.07	-2.23	66,66,66,66	0
10	MG	D	2001	1/1	0.97	0.10	-2.38	81,81,81,81	0
10	MG	B	2001	1/1	0.97	0.09	-2.73	61,61,61,61	0
6	CA	B	2003	1/1	0.94	0.04	-5.17	120,120,120,120	0
11	NAG	D	3080	14/15	0.76	0.25	-	101,123,128,129	0
11	NAG	D	3243	14/15	0.78	0.21	-	100,134,147,151	0
5	SO4	C	1596	5/5	0.96	0.08	-	107,107,109,109	5
11	NAG	C	3524	14/15	0.77	0.35	-	116,136,158,159	0
5	SO4	B	1475	5/5	0.71	0.37	-	235,237,244,245	0
11	NAG	B	3243	14/15	0.87	0.18	-	105,111,118,120	0
5	SO4	A	1595	5/5	0.99	0.11	-	47,47,52,53	5
13	MAN	C	3461	11/12	0.85	0.17	-	98,105,113,115	0
11	NAG	B	3080	14/15	0.84	0.40	-	109,130,164,168	0
11	NAG	D	3031	14/15	0.74	0.48	-	116,141,156,158	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.