



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:01 AM GMT

PDB ID : 3V4P
Title : crystal structure of a4b7 headpiece complexed with Fab ACT-1
Authors : Yu, Y.; Zhu, J.; Springer, T.A.
Deposited on : 2011-12-15
Resolution : 3.15 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

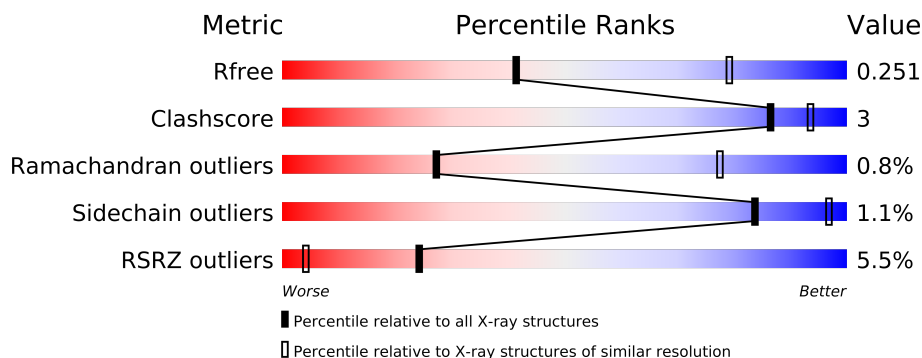
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.15 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}	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	597	
1	C	597	
2	B	503	
2	D	503	
3	H	219	
3	M	219	
4	L	217	
4	N	217	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	A	605	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	15P	A	612	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21722 atoms, of which 0 are hydrogen and 0 are deuterium.

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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	14	0	0
			4493	2834	773	864	22			
1	C	581	Total	C	N	O	S	19	0	0
			4496	2835	776	863	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ALA	ARG	ENGINEERED MUTATION	UNP P13612
A	588	THR	-	EXPRESSION TAG	UNP P13612
A	589	GLY	-	EXPRESSION TAG	UNP P13612
A	590	GLY	-	EXPRESSION TAG	UNP P13612
A	591	LEU	-	EXPRESSION TAG	UNP P13612
A	592	GLU	-	EXPRESSION TAG	UNP P13612
A	593	ASN	-	EXPRESSION TAG	UNP P13612
A	594	LEU	-	EXPRESSION TAG	UNP P13612
A	595	TYR	-	EXPRESSION TAG	UNP P13612
A	596	PHE	-	EXPRESSION TAG	UNP P13612
A	597	GLN	-	EXPRESSION TAG	UNP P13612
C	558	ALA	ARG	ENGINEERED MUTATION	UNP P13612
C	588	THR	-	EXPRESSION TAG	UNP P13612
C	589	GLY	-	EXPRESSION TAG	UNP P13612
C	590	GLY	-	EXPRESSION TAG	UNP P13612
C	591	LEU	-	EXPRESSION TAG	UNP P13612
C	592	GLU	-	EXPRESSION TAG	UNP P13612
C	593	ASN	-	EXPRESSION TAG	UNP P13612
C	594	LEU	-	EXPRESSION TAG	UNP P13612
C	595	TYR	-	EXPRESSION TAG	UNP P13612
C	596	PHE	-	EXPRESSION TAG	UNP P13612
C	597	GLN	-	EXPRESSION TAG	UNP P13612

- Molecule 2 is a protein called Integrin beta-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	6	2	0
			2922	1828	519	563	12			
2	D	375	Total	C	N	O	S	0	1	0
			2916	1824	518	562	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	494	SER	-	EXPRESSION TAG	UNP P26010
B	495	ARG	-	EXPRESSION TAG	UNP P26010
B	496	GLY	-	EXPRESSION TAG	UNP P26010
B	497	LEU	-	EXPRESSION TAG	UNP P26010
B	498	GLU	-	EXPRESSION TAG	UNP P26010
B	499	ASN	-	EXPRESSION TAG	UNP P26010
B	500	LEU	-	EXPRESSION TAG	UNP P26010
B	501	TYR	-	EXPRESSION TAG	UNP P26010
B	502	PHE	-	EXPRESSION TAG	UNP P26010
B	503	GLN	-	EXPRESSION TAG	UNP P26010
D	494	SER	-	EXPRESSION TAG	UNP P26010
D	495	ARG	-	EXPRESSION TAG	UNP P26010
D	496	GLY	-	EXPRESSION TAG	UNP P26010
D	497	LEU	-	EXPRESSION TAG	UNP P26010
D	498	GLU	-	EXPRESSION TAG	UNP P26010
D	499	ASN	-	EXPRESSION TAG	UNP P26010
D	500	LEU	-	EXPRESSION TAG	UNP P26010
D	501	TYR	-	EXPRESSION TAG	UNP P26010
D	502	PHE	-	EXPRESSION TAG	UNP P26010
D	503	GLN	-	EXPRESSION TAG	UNP P26010

- Molecule 3 is a protein called MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	211	Total	C	N	O	S	0	0	0
			1607	1021	258	321	7			
3	M	211	Total	C	N	O	S	0	0	0
			1607	1021	258	321	7			

- Molecule 4 is a protein called MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	217	Total	C	N	O	S	0	0	0
			1681	1054	282	339	6			

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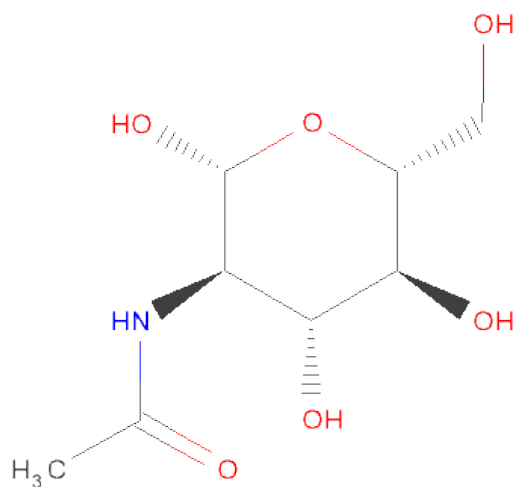
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	217	Total	C	N	O	S	0	0	0
			1681	1054	282	339	6			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	3	Total	Ca	0	0
			3	3		
5	D	2	Total	Ca	0	0
			2	2		
5	C	3	Total	Ca	0	0
			3	3		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

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

There are 22 discrepancies between the modelled and reference sequences:

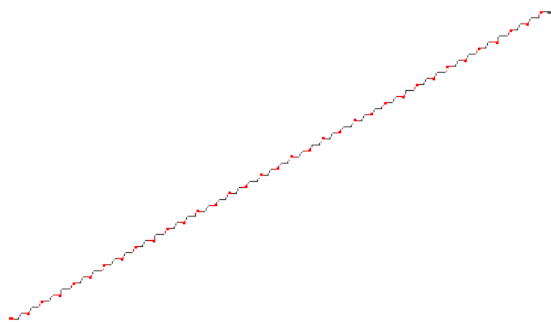
Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ALA	ARG	ENGINEERED MUTATION	UNP P13612
A	588	THR	-	EXPRESSION TAG	UNP P13612
A	589	GLY	-	EXPRESSION TAG	UNP P13612
A	590	GLY	-	EXPRESSION TAG	UNP P13612
A	591	LEU	-	EXPRESSION TAG	UNP P13612
A	592	GLU	-	EXPRESSION TAG	UNP P13612
A	593	ASN	-	EXPRESSION TAG	UNP P13612
A	594	LEU	-	EXPRESSION TAG	UNP P13612
A	595	TYR	-	EXPRESSION TAG	UNP P13612
A	596	PHE	-	EXPRESSION TAG	UNP P13612
A	597	GLN	-	EXPRESSION TAG	UNP P13612
C	558	ALA	ARG	ENGINEERED MUTATION	UNP P13612
C	588	THR	-	EXPRESSION TAG	UNP P13612
C	589	GLY	-	EXPRESSION TAG	UNP P13612
C	590	GLY	-	EXPRESSION TAG	UNP P13612
C	591	LEU	-	EXPRESSION TAG	UNP P13612
C	592	GLU	-	EXPRESSION TAG	UNP P13612
C	593	ASN	-	EXPRESSION TAG	UNP P13612
C	594	LEU	-	EXPRESSION TAG	UNP P13612
C	595	TYR	-	EXPRESSION TAG	UNP P13612

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Chain	Residue	Modelled	Actual	Comment	Reference
C	596	PHE	-	EXPRESSION TAG	UNP P13612
C	597	GLN	-	EXPRESSION TAG	UNP P13612

- Molecule 8 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: C₆₉H₁₄₀O₃₅).

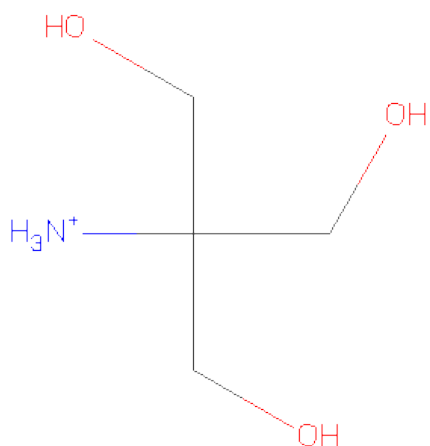


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			52	34	18		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 11 is water.

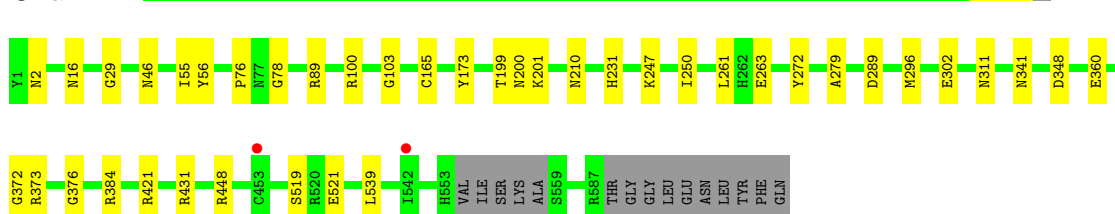
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	O	0	0
			4	4		
11	B	7	Total	O	0	0
			7	7		
11	C	3	Total	O	0	0
			3	3		
11	D	7	Total	O	0	0
			7	7		

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.

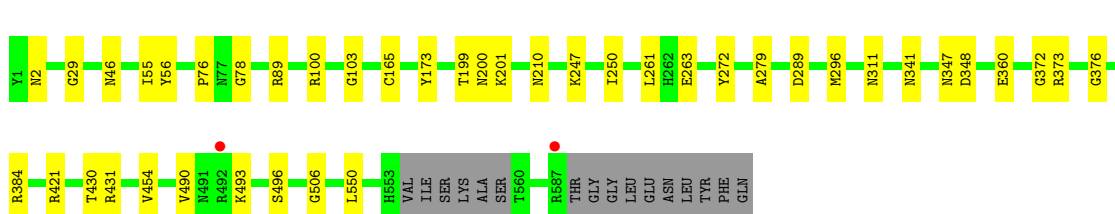
• Molecule 1: Integrin alpha-4

Chain A:



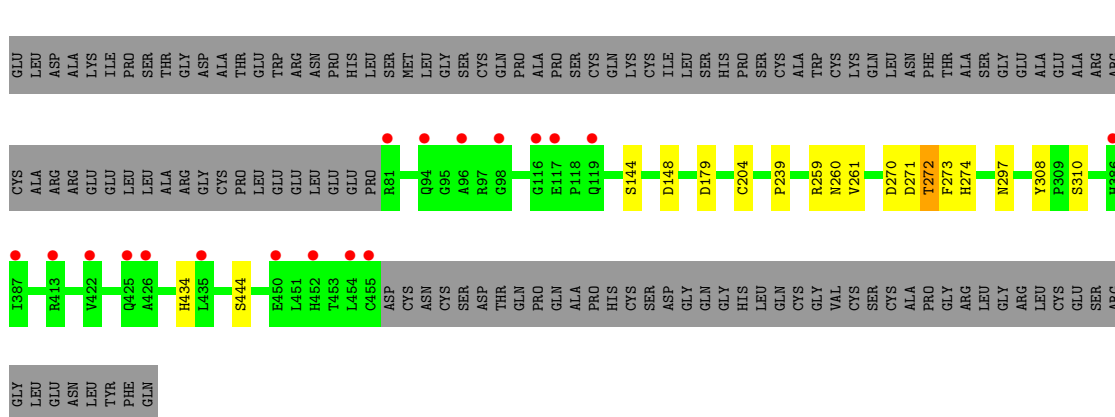
• Molecule 1: Integrin alpha-4

Chain C:



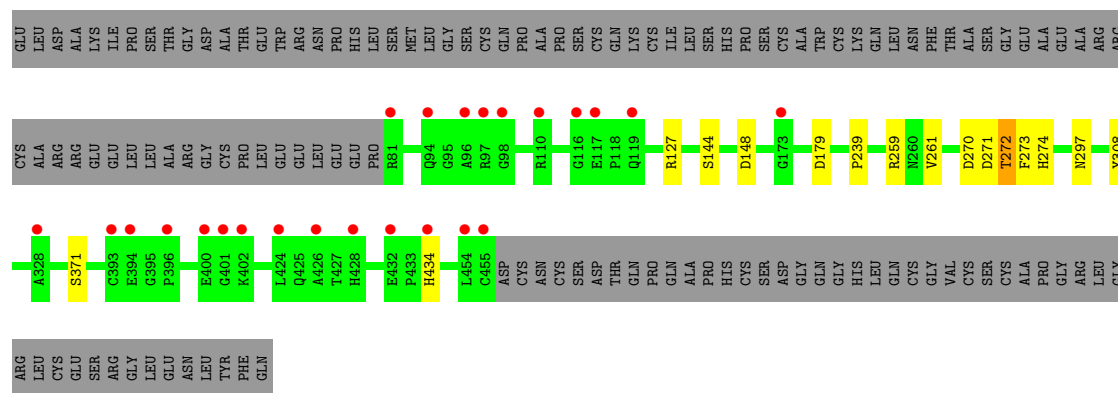
• Molecule 2: Integrin beta-7

Chain B:



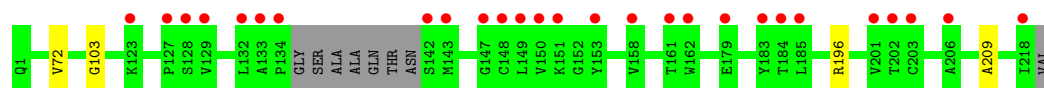
• Molecule 2: Integrin beta-7

Chain D:



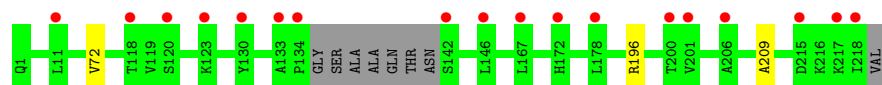
• Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN

Chain H:



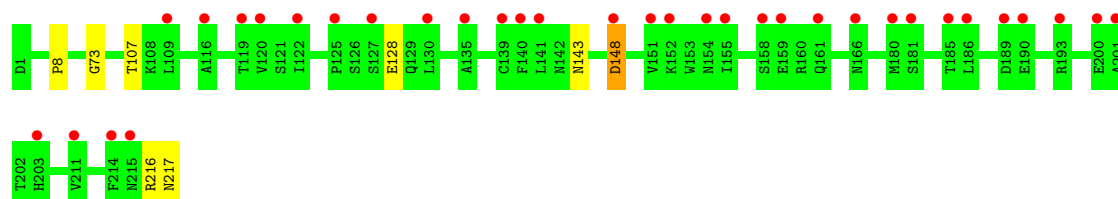
• Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN

Chain M:



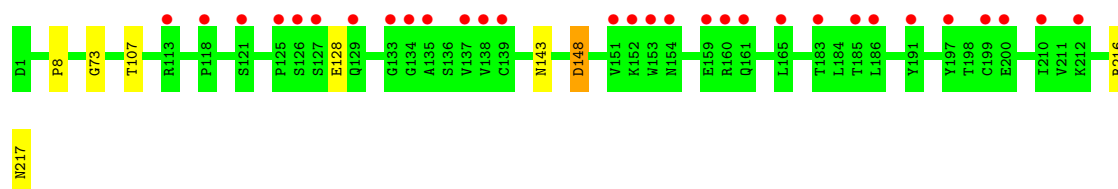
• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN

Chain L:



• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.78Å 122.74Å 158.14Å 90.00° 115.38° 90.00°	Depositor
Resolution (Å)	46.13 – 3.15 46.13 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.13-3.15) 97.4 (46.13-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.220 , 0.251 0.218 , 0.251	Depositor DCC
R_{free} test set	1066 reflections (1.30%)	DCC
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 93.7	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 82061 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	21722	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 15P, MG, BMA, NAG, CA, TRS, 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	0.25	0/4593	0.45	1/6221 (0.0%)
1	C	0.25	0/4596	0.45	1/6224 (0.0%)
2	B	0.23	0/2984	0.41	0/4053
2	D	0.23	0/2978	0.41	0/4044
3	H	0.22	0/1652	0.40	0/2259
3	M	0.22	0/1652	0.40	0/2259
4	L	0.22	0/1722	0.38	0/2340
4	N	0.22	0/1722	0.38	0/2340
All	All	0.23	0/21899	0.42	2/29740 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	348	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4493	0	0	19	0
1	C	4496	0	0	18	0
2	B	2922	0	0	8	0
2	D	2916	0	0	6	0
3	H	1607	0	0	1	0
3	M	1607	0	0	0	0
4	L	1681	0	18	4	0
4	N	1681	0	18	4	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
6	A	56	0	52	1	0
6	B	14	0	13	0	0
6	C	56	0	52	1	0
7	A	50	0	43	1	0
7	C	50	0	43	0	0
8	A	52	0	69	3	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	8	0	12	0	0
11	A	4	0	0	2	0
11	B	7	0	0	0	0
11	C	3	0	0	3	0
11	D	7	0	0	0	0
All	All	21722	0	320	58	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:372:GLY:O	11:A:702:HOH:O	1.99	0.79
1:A:311:ASN:O	11:A:701:HOH:O	2.07	0.71
1:C:372:GLY:O	11:C:702:HOH:O	2.13	0.67
1:C:430:THR:N	11:C:703:HOH:O	2.27	0.67
1:A:199:THR:O	1:A:201:LYS:N	2.31	0.63
1:C:199:THR:O	1:C:201:LYS:N	2.32	0.63
2:B:144:SER:OG	2:B:270:ASP:OD2	2.20	0.59
2:D:144:SER:OG	2:D:270:ASP:OD2	2.21	0.58
1:C:311:ASN:O	11:C:701:HOH:O	2.18	0.57
4:L:216:ARG:HG2	4:L:217:ASN:H	1.71	0.56
4:N:148:ASP:N	4:N:148:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:100:ARG:NH2	1:A:103:GLY:O	2.40	0.55
4:L:148:ASP:OD1	4:L:148:ASP:N	2.39	0.55
2:B:260:ASN:OD1	2:B:444:SER:OG	2.25	0.54
1:C:100:ARG:NH2	1:C:103:GLY:O	2.40	0.54
2:B:179:ASP:OD1	2:B:308:TYR:OH	2.26	0.54
1:A:56:TYR:CE2	8:A:612:15P:H191	2.42	0.54
1:C:493:LYS:NZ	1:C:496:SER:O	2.40	0.54
2:D:179:ASP:OD1	2:D:308:TYR:OH	2.26	0.53
1:C:89:ARG:NH2	6:C:604:NAG:O6	2.42	0.52
4:N:216:ARG:HG2	4:N:217:ASN:H	1.75	0.51
2:D:127:ARG:NH2	2:D:371:SER:OG	2.44	0.50
4:L:8:PRO:O	4:L:107:THR:OG1	2.30	0.50
4:N:8:PRO:O	4:N:107:THR:OG1	2.30	0.50
1:C:2:ASN:O	1:C:431:ARG:N	2.45	0.50
1:A:210:ASN:ND2	1:A:210:ASN:O	2.45	0.50
1:A:231:HIS:CD2	7:A:609:MAN:H62	2.47	0.49
2:D:272:THR:OG1	2:D:273:PHE:N	2.45	0.49
1:A:289:ASP:OD1	1:A:311:ASN:N	2.45	0.49
1:C:289:ASP:OD1	1:C:311:ASN:N	2.45	0.49
1:A:16:ASN:ND2	8:A:612:15P:H252	2.27	0.49
1:A:2:ASN:O	1:A:431:ARG:N	2.46	0.48
1:C:210:ASN:ND2	1:C:210:ASN:O	2.47	0.47
1:A:519:SER:O	1:A:521:GLU:N	2.48	0.47
1:A:247:LYS:NZ	1:A:263:GLU:OE2	2.47	0.46
1:A:302:GLU:OE1	2:B:310:SER:OG	2.33	0.46
1:C:247:LYS:NZ	1:C:263:GLU:OE2	2.48	0.46
1:C:46:ASN:ND2	1:C:76:PRO:O	2.50	0.45
1:A:373:ARG:N	1:A:376:GLY:O	2.49	0.44
2:B:272[A]:THR:OG1	2:B:273:PHE:N	2.50	0.44
1:C:373:ARG:N	1:C:376:GLY:O	2.51	0.44
1:C:279:ALA:O	1:C:341:ASN:ND2	2.49	0.44
1:C:360:GLU:OE1	1:C:384:ARG:NH2	2.51	0.43
2:B:204:CYS:N	3:H:103:GLY:O	2.52	0.43
1:A:279:ALA:O	1:A:341:ASN:ND2	2.51	0.43
1:A:46:ASN:ND2	1:A:76:PRO:O	2.50	0.43
1:A:89:ARG:NH2	6:A:604:NAG:O6	2.51	0.43
1:A:360:GLU:OE1	1:A:384:ARG:NH2	2.51	0.43
2:D:259:ARG:O	2:D:261:VAL:N	2.53	0.42
2:D:239:PRO:O	2:D:274:HIS:CD2	2.73	0.42
2:B:259:ARG:O	2:B:261:VAL:N	2.52	0.42
8:A:612:15P:H142	1:C:56:TYR:CE2	2.55	0.42
4:N:128:GLU:N	4:N:128:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:250:ILE:O	1:A:261:LEU:N	2.54	0.41
4:L:128:GLU:N	4:L:128:GLU:OE1	2.53	0.41
1:C:250:ILE:O	1:C:261:LEU:N	2.54	0.41
2:B:239:PRO:O	2:B:274:HIS:CD2	2.74	0.40
1:C:347:ASN:ND2	1:C:347:ASN:O	2.55	0.40

There are no symmetry-related clashes.

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	578/597 (97%)	520 (90%)	53 (9%)	5 (1%)	25	75
1	C	577/597 (97%)	523 (91%)	48 (8%)	6 (1%)	22	73
2	B	375/503 (75%)	328 (88%)	44 (12%)	3 (1%)	27	77
2	D	374/503 (74%)	330 (88%)	42 (11%)	2 (0%)	38	85
3	H	207/219 (94%)	186 (90%)	20 (10%)	1 (0%)	38	85
3	M	207/219 (94%)	186 (90%)	20 (10%)	1 (0%)	38	85
4	L	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	25	75
4	N	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	25	75
All	All	2748/3072 (90%)	2475 (90%)	251 (9%)	22 (1%)	27	77

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	C	200	ASN
4	L	73	GLY
4	N	73	GLY
1	A	29	GLY
1	A	448	ARG
1	C	29	GLY

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Mol	Chain	Res	Type
2	D	272	THR
1	A	539	LEU
2	B	434	HIS
2	D	434	HIS
3	H	209	ALA
4	L	143	ASN
3	M	209	ALA
4	N	143	ASN
2	B	272[A]	THR
2	B	272[B]	THR
1	C	454	VAL
1	C	490	VAL
1	C	506	GLY
1	A	78	GLY
1	C	78	GLY

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	486/500 (97%)	480 (99%)	6 (1%)	82	96
1	C	487/500 (97%)	480 (99%)	7 (1%)	78	95
2	B	325/431 (75%)	321 (99%)	4 (1%)	82	96
2	D	324/431 (75%)	320 (99%)	4 (1%)	82	96
3	H	183/188 (97%)	181 (99%)	2 (1%)	84	97
3	M	183/188 (97%)	181 (99%)	2 (1%)	84	97
4	L	194/194 (100%)	193 (100%)	1 (0%)	94	99
4	N	194/194 (100%)	193 (100%)	1 (0%)	94	99
All	All	2376/2626 (90%)	2349 (99%)	27 (1%)	84	97

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	165	CYS

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Mol	Chain	Res	Type
1	A	173	TYR
1	A	272	TYR
1	A	296	MET
1	A	421	ARG
2	B	148	ASP
2	B	271[A]	ASP
2	B	271[B]	ASP
2	B	297	ASN
1	C	55	ILE
1	C	165	CYS
1	C	173	TYR
1	C	272	TYR
1	C	296	MET
1	C	421	ARG
1	C	550	LEU
2	D	148	ASP
2	D	271[A]	ASP
2	D	271[B]	ASP
2	D	297	ASN
3	H	72	VAL
3	H	196	ARG
4	L	148	ASP
3	M	72	VAL
3	M	196	ARG
4	N	148	ASP

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

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 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	606	1,7	12,14,15	0.77	1 (8%)	15,19,21	0.77	0
7	NAG	A	607	7	12,14,15	0.69	1 (8%)	15,19,21	0.91	1 (6%)
7	BMA	A	608	7	10,11,12	0.94	1 (10%)	11,15,17	1.73	3 (27%)
7	MAN	A	609	7	10,11,12	0.62	0	11,15,17	0.83	1 (9%)
7	NAG	C	606	1,7	12,14,15	0.72	1 (8%)	15,19,21	1.22	1 (6%)
7	NAG	C	607	7	12,14,15	0.79	1 (8%)	15,19,21	1.08	1 (6%)
7	BMA	C	608	7	10,11,12	0.77	0	11,15,17	1.06	1 (9%)
7	MAN	C	609	7	10,11,12	0.85	1 (10%)	11,15,17	0.90	1 (9%)

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	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	607	7	-	0/6/23/26	0/1/1/1
7	BMA	A	608	7	-	0/2/19/22	0/1/1/1
7	MAN	A	609	7	-	0/2/19/22	0/1/1/1
7	NAG	C	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	607	7	-	0/6/23/26	0/1/1/1
7	BMA	C	608	7	-	0/2/19/22	0/1/1/1
7	MAN	C	609	7	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	608	BMA	O5-C5	-2.55	1.40	1.45
7	A	606	NAG	O5-C5	-2.41	1.40	1.45
7	C	607	NAG	O5-C5	-2.30	1.41	1.45
7	C	606	NAG	O5-C5	-2.24	1.41	1.45
7	C	609	MAN	O5-C5	-2.18	1.41	1.45
7	A	607	NAG	O5-C5	-2.10	1.41	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	608	BMA	C4-C3-C2	4.18	116.11	110.50
7	A	608	BMA	O5-C5-C4	-2.88	107.00	110.65
7	C	608	BMA	O5-C5-C6	2.74	109.85	106.98
7	C	606	NAG	C3-C4-C5	2.53	114.72	110.20
7	C	607	NAG	O5-C5-C6	2.44	109.55	106.98
7	A	607	NAG	O5-C5-C6	2.33	109.42	106.98
7	C	609	MAN	O5-C5-C6	2.27	109.36	106.98
7	A	609	MAN	O5-C5-C4	2.20	113.45	110.65
7	A	608	BMA	O5-C5-C6	2.20	109.29	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 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	$\# Z > 2$
6	NAG	A	604	1	12,14,15	0.71	1 (8%)	15,19,21	1.03	1 (6%)
6	NAG	A	605	1	12,14,15	0.69	1 (8%)	15,19,21	0.78	0
6	NAG	A	610	1	12,14,15	0.70	1 (8%)	15,19,21	0.82	0
6	NAG	A	611	1	12,14,15	0.63	0	15,19,21	0.97	1 (6%)
8	15P	A	612	-	51,51,103	0.54	0	50,50,102	1.48	2 (4%)
6	NAG	B	2004	2	12,14,15	0.86	1 (8%)	15,19,21	0.87	0
6	NAG	C	604	1	12,14,15	0.74	1 (8%)	15,19,21	0.95	0
6	NAG	C	605	1	12,14,15	0.70	1 (8%)	15,19,21	0.76	1 (6%)
6	NAG	C	610	1	12,14,15	0.65	0	15,19,21	0.91	1 (6%)
6	NAG	C	611	1	12,14,15	0.61	0	15,19,21	0.75	0
10	TRS	C	612	-	7,7,7	2.23	1 (14%)	9,9,9	1.64	3 (33%)

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
6	NAG	A	604	1	-	0/6/23/26	0/1/1/1
6	NAG	A	605	1	-	0/6/23/26	0/1/1/1
6	NAG	A	610	1	-	0/6/23/26	0/1/1/1
6	NAG	A	611	1	-	0/6/23/26	0/1/1/1
8	15P	A	612	-	-	0/49/49/101	0/0/0/0
6	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
6	NAG	C	604	1	-	0/6/23/26	0/1/1/1
6	NAG	C	605	1	-	0/6/23/26	0/1/1/1
6	NAG	C	610	1	-	0/6/23/26	0/1/1/1
6	NAG	C	611	1	-	0/6/23/26	0/1/1/1
10	TRS	C	612	-	-	0/9/9/9	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	612	TRS	C-N	-4.86	1.43	1.50
6	C	604	NAG	O5-C5	-2.22	1.41	1.45
6	C	605	NAG	O5-C5	-2.17	1.41	1.45
6	A	605	NAG	O5-C5	-2.16	1.41	1.45
6	A	604	NAG	O5-C5	-2.12	1.41	1.45
6	A	610	NAG	O5-C5	-2.10	1.41	1.45
6	B	2004	NAG	O5-C5	-2.06	1.41	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	612	TRS	O1-C1-C	3.00	118.13	111.55
6	A	604	NAG	O5-C5-C6	2.85	109.97	106.98
6	C	610	NAG	O5-C5-C6	2.64	109.75	106.98
10	C	612	TRS	O3-C3-C	2.56	117.16	111.55
10	C	612	TRS	O2-C2-C	2.54	117.11	111.55
6	A	611	NAG	O5-C5-C6	2.53	109.64	106.98
8	A	612	15P	O11-C23-C24	2.03	119.69	110.47
8	A	612	15P	O15-C30-C29	2.02	119.62	110.47
6	C	605	NAG	O5-C5-C6	2.01	109.09	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	582/597 (97%)	0.25	2 (0%)	91 56	38, 89, 161, 227	3 (0%)
1	C	581/597 (97%)	0.23	2 (0%)	91 56	47, 96, 166, 236	4 (0%)
2	B	375/503 (74%)	0.50	18 (4%)	29 5	51, 126, 203, 263	0
2	D	375/503 (74%)	0.53	24 (6%)	19 3	69, 131, 198, 240	0
3	H	211/219 (96%)	0.77	27 (12%)	4 1	83, 168, 230, 247	0
3	M	211/219 (96%)	0.86	18 (8%)	11 2	101, 176, 231, 246	0
4	L	217/217 (100%)	1.05	34 (15%)	3 1	93, 167, 249, 274	0
4	N	217/217 (100%)	0.91	30 (13%)	4 1	102, 168, 251, 276	0
All	All	2769/3072 (90%)	0.52	155 (5%)	24 4	38, 125, 224, 276	7 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	455	CYS	11.2
4	L	135	ALA	8.9
2	D	97	ARG	8.7
4	N	186	LEU	8.2
4	N	134	GLY	7.5
4	N	135	ALA	7.4
4	N	197	TYR	7.1
4	L	159	GLU	6.9
3	H	133	ALA	6.5
4	N	160	ARG	6.1
2	B	425	GLN	6.0
4	N	185	THR	5.6
2	D	455	CYS	5.6
2	B	454	LEU	5.6
3	H	218	ILE	5.3
4	N	183	THR	5.2

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Mol	Chain	Res	Type	RSRZ
4	N	199	CYS	5.2
4	L	180	MET	5.0
3	H	206	ALA	5.0
3	M	146	LEU	4.8
1	C	492	ARG	4.8
4	L	189	ASP	4.7
3	M	215	ASP	4.7
4	L	141	LEU	4.7
3	M	133	ALA	4.5
4	N	212	LYS	4.3
4	L	152	LYS	4.3
4	N	125	PRO	4.3
2	B	81	ARG	4.3
2	D	96	ALA	4.2
2	D	98	GLY	4.2
3	M	134	PRO	4.0
4	L	203	HIS	4.0
2	D	454	LEU	4.0
4	L	193	ARG	4.0
4	L	185	THR	4.0
4	L	125	PRO	3.9
2	D	394	GLU	3.8
4	N	159	GLU	3.8
2	B	116	GLY	3.7
3	H	184	THR	3.7
2	B	435	LEU	3.6
4	L	201	ALA	3.6
2	B	426	ALA	3.6
2	D	117	GLU	3.5
4	L	154	ASN	3.5
3	H	202	THR	3.5
2	D	428	HIS	3.5
4	N	200	GLU	3.5
3	M	11	LEU	3.5
2	D	116	GLY	3.4
3	H	123	LYS	3.4
3	M	167	LEU	3.4
3	M	142	SER	3.3
4	L	200	GLU	3.2
3	H	179	GLU	3.2
2	B	94	GLN	3.2
4	L	186	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
4	L	215	ASN	3.2
4	L	139	CYS	3.2
4	L	190	GLU	3.1
2	B	386	HIS	3.1
2	B	452	HIS	3.1
3	H	185	LEU	3.1
3	H	147	GLY	3.1
3	H	149	LEU	3.0
4	L	158	SER	3.0
4	N	129	GLN	3.0
2	D	432	GLU	3.0
4	N	152	LYS	3.0
4	L	148	ASP	2.9
2	D	110	ARG	2.9
4	L	109	LEU	2.9
4	L	214	PHE	2.9
2	B	387	ILE	2.9
4	L	127	SER	2.9
2	D	393	CYS	2.9
4	N	165	LEU	2.9
4	N	210	ILE	2.8
2	D	424	LEU	2.8
2	B	117	GLU	2.8
2	D	400	GLU	2.8
4	N	139	CYS	2.8
2	B	98	GLY	2.8
3	H	151	LYS	2.8
2	D	426	ALA	2.8
3	H	127	PRO	2.8
3	H	132	LEU	2.8
3	H	150	VAL	2.8
3	H	183	TYR	2.7
3	M	120	SER	2.7
4	N	154	ASN	2.7
4	L	140	PHE	2.7
4	L	116	ALA	2.7
3	M	217	LYS	2.7
3	M	200	THR	2.7
3	H	161	THR	2.7
2	D	401	GLY	2.7
3	M	123	LYS	2.6
2	D	434	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	422	VAL	2.6
2	D	81	ARG	2.6
4	L	120	VAL	2.6
4	N	118	PRO	2.5
3	H	129	VAL	2.5
3	M	218	ILE	2.5
2	B	96	ALA	2.5
3	H	162	TRP	2.5
3	H	153	TYR	2.5
3	H	143	MET	2.4
2	B	450	GLU	2.4
4	L	166	ASN	2.4
3	H	158	VAL	2.4
3	M	178	LEU	2.4
2	D	402	LYS	2.4
4	L	119	THR	2.4
4	N	133	GLY	2.4
4	N	127	SER	2.4
3	M	201	VAL	2.4
3	H	201	VAL	2.3
4	L	155	ILE	2.3
3	H	128	SER	2.3
4	N	138	VAL	2.3
2	B	413	ARG	2.3
4	N	161	GLN	2.3
3	H	142	SER	2.3
4	N	153	TRP	2.3
3	M	130	TYR	2.3
4	N	126	SER	2.3
3	M	172	HIS	2.2
2	D	94	GLN	2.2
2	B	119	GLN	2.2
4	L	122	ILE	2.2
4	L	130	LEU	2.2
2	D	119	GLN	2.2
3	M	118	THR	2.2
3	H	148	CYS	2.2
1	A	453	CYS	2.2
3	H	203	CYS	2.2
4	N	113	ARG	2.2
4	N	121	SER	2.2
1	A	542	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	396	PRO	2.1
1	C	587	ARG	2.1
4	N	191	TYR	2.1
2	D	173	GLY	2.1
4	L	181	SER	2.1
4	L	161	GLN	2.0
4	N	151	VAL	2.0
4	L	151	VAL	2.0
4	L	211	VAL	2.0
2	D	328	ALA	2.0
4	N	137	VAL	2.0
3	M	206	ALA	2.0
3	H	134	PRO	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 ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MAN	A	609	11/12	0.45	0.01	115,192,228,245	0
7	NAG	C	606	14/15	0.25	-0.24	60,152,181,188	0
7	NAG	A	607	14/15	0.23	-0.80	58,121,166,179	0
7	NAG	A	606	14/15	0.24	-1.07	45,111,145,158	0
7	BMA	A	608	11/12	0.19	-2.77	112,197,215,224	0
7	BMA	C	608	11/12	0.21	-	182,203,226,244	0
7	NAG	C	607	14/15	0.18	-	130,154,204,205	0
7	MAN	C	609	11/12	0.53	-	180,237,249,252	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	A	605	14/15	0.30	3.62	67,160,177,193	0
8	15P	A	612	52/104	0.41	2.92	3,88,137,176	0
10	TRS	C	612	8/8	0.38	1.76	114,148,166,167	0
5	CA	C	603	1/1	0.34	1.67	68,68,68,68	0
9	MG	B	2001	1/1	0.31	0.74	100,100,100,100	0
5	CA	A	603	1/1	0.28	0.72	69,69,69,69	0
6	NAG	A	611	14/15	0.29	0.55	110,149,210,214	0
6	NAG	A	610	14/15	0.26	0.21	133,157,188,195	0
5	CA	A	602	1/1	0.27	0.10	78,78,78,78	0
6	NAG	C	610	14/15	0.33	-0.06	119,164,193,202	0
6	NAG	A	604	14/15	0.26	-0.46	47,75,103,114	0
6	NAG	C	611	14/15	0.27	-0.49	135,147,173,176	0
6	NAG	B	2004	14/15	0.25	-0.57	143,177,230,235	0
6	NAG	C	604	14/15	0.24	-0.58	52,87,127,156	0
5	CA	A	601	1/1	0.23	-0.69	81,81,81,81	0
5	CA	B	2003	1/1	0.24	-0.76	87,87,87,87	0
6	NAG	C	605	14/15	0.21	-0.80	69,157,189,199	0
5	CA	C	601	1/1	0.25	-0.81	86,86,86,86	0
5	CA	C	602	1/1	0.23	-0.86	86,86,86,86	0
9	MG	D	2001	1/1	0.17	-1.28	104,104,104,104	0
5	CA	D	2002	1/1	0.18	-1.50	132,132,132,132	0
5	CA	D	2003	1/1	0.15	-2.20	115,115,115,115	0
5	CA	B	2002	1/1	0.08	-2.66	125,125,125,125	0

6.5 Other polymers ⓘ

There are no such residues in this entry.