



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:05 AM BST

PDB ID : 3K2U  
Title : Crystal structure of HGFA in complex with the allosteric inhibitory antibody Fab40  
Authors : Ganesan, R.; Eigenbrot, C.; Shia, S.  
Deposited on : 2009-09-30  
Resolution : 2.35 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

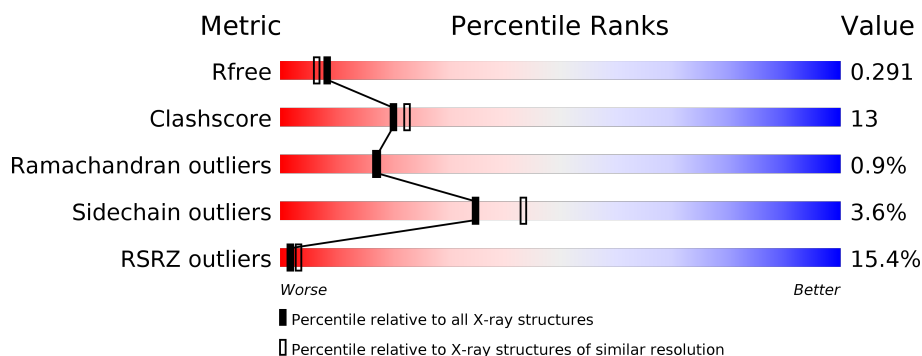
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	<div> <div>18%</div> <div>68%</div> <div>21%</div> <div>• 9%</div> </div>
2	B	35	<div> <div>6%</div> <div>9%</div> <div>6%</div> <div>86%</div> </div>
3	H	225	<div> <div>12%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
4	L	214	<div> <div>13%</div> <div>64%</div> <div>31%</div> <div>• •</div> </div>
5	C	2	<div> <div>50%</div> <div>50%</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
5	NAG	C	2	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5207 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 Hepatocyte growth factor activator long chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1780	1133	306	328	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	ALA	-	expression tag	UNP Q04756
A	254	ALA	-	expression tag	UNP Q04756
A	255	ALA	-	expression tag	UNP Q04756
A	256	HIS	-	expression tag	UNP Q04756
A	257	HIS	-	expression tag	UNP Q04756
A	258	HIS	-	expression tag	UNP Q04756
A	259	HIS	-	expression tag	UNP Q04756
A	260	HIS	-	expression tag	UNP Q04756
A	261	HIS	-	expression tag	UNP Q04756

- Molecule 2 is a protein called Hepatocyte growth factor activator short chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	S	0	0	0
			37	20	11	5	1			

- Molecule 3 is a protein called Antibody, Fab fragment, Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1603	1024	265	308	6			

- Molecule 4 is a protein called Antibody, Fab fragment, Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	208	Total	C	N	O	S	0	0	0
			1591	994	267	324	6			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

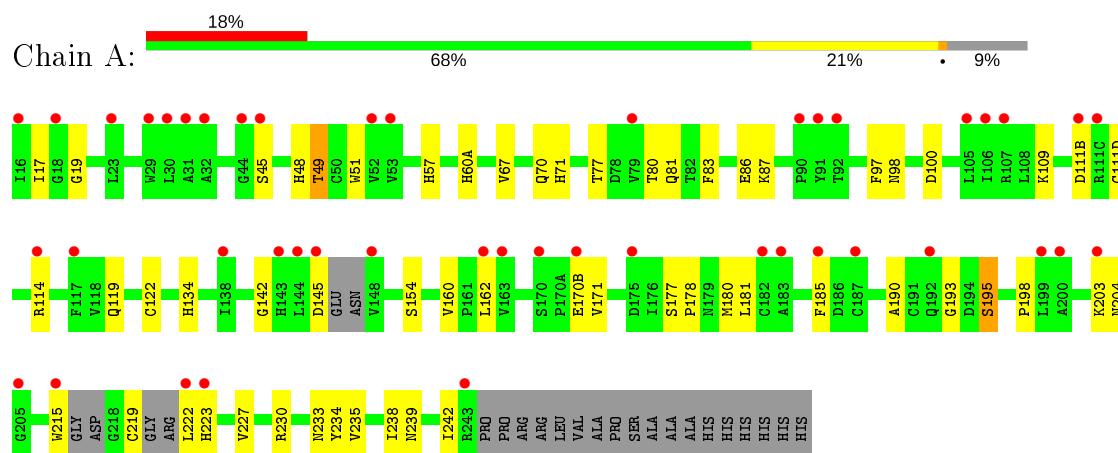
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total	O	0	0
			72	72		
6	B	2	Total	O	0	0
			2	2		
6	H	54	Total	O	0	0
			54	54		
6	L	40	Total	O	0	0
			40	40		

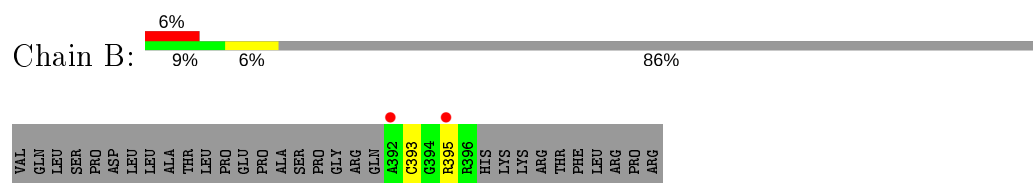
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

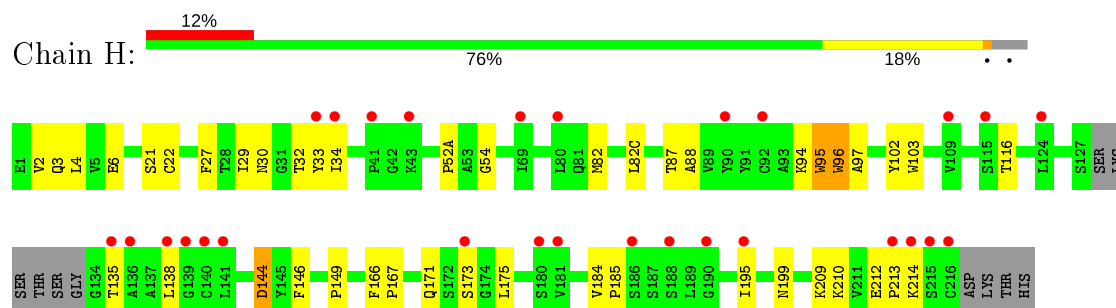
- Molecule 1: Hepatocyte growth factor activator long chain



- Molecule 2: Hepatocyte growth factor activator short chain

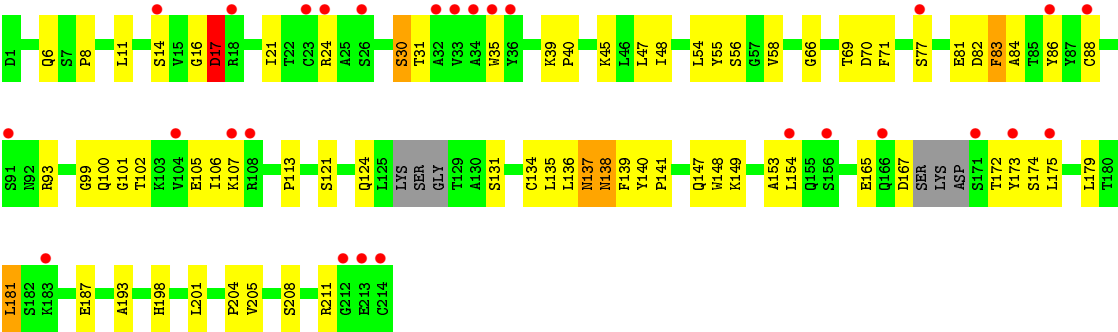


- Molecule 3: Antibody, Fab fragment, Heavy Chain



- Molecule 4: Antibody, Fab fragment, Light Chain





● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.94Å 48.93Å 96.03Å 98.10° 95.01° 103.89°	Depositor
Resolution (Å)	19.77 – 2.35 19.77 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.8 (19.77-2.35) 94.9 (19.77-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 2.35Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239 , 0.290 0.239 , 0.291	Depositor DCC
$R_{free}$ test set	2653 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.47	2/1831 (0.1%)	0.60	0/2491
2	B	0.46	0/36	0.70	0/45
3	H	0.45	0/1648	0.64	0/2253
4	L	0.39	0/1623	0.58	0/2202
All	All	0.44	2/5138 (0.0%)	0.61	0/6991

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	ILE	C-N	8.15	1.47	1.33
1	A	19	GLY	C-N	5.43	1.46	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1780	0	1699	37	0
2	B	37	0	37	1	0
3	H	1603	0	1558	33	0
4	L	1591	0	1540	55	0
5	C	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	72	0	0	4	0
6	B	2	0	0	0	0
6	H	54	0	0	1	0
6	L	40	0	0	2	0
All	All	5207	0	4859	124	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 13.

All (124) 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)
6:A:312:HOH:O	5:C:1:NAG:O6	1.71	1.07
4:L:47:LEU:HD22	4:L:58:VAL:HG13	1.67	0.76
1:A:86:GLU:OE2	1:A:109:LYS:HG2	1.87	0.73
4:L:179:LEU:HG	4:L:181:LEU:HD11	1.75	0.68
4:L:105:GLU:HG2	4:L:106:ILE:N	2.09	0.67
1:A:45:SER:OG	1:A:198:PRO:HB3	1.95	0.67
4:L:6:GLN:HB2	4:L:100:GLN:NE2	2.10	0.67
4:L:11:LEU:O	4:L:11:LEU:HD12	1.95	0.67
3:H:30:ASN:HA	3:H:52(A):PRO:HB2	1.77	0.66
3:H:4:LEU:HD12	3:H:22:CYS:SG	2.36	0.66
1:A:230:ARG:HD2	1:A:233:ASN:ND2	2.11	0.64
1:A:134:HIS:HB3	1:A:162:LEU:HD12	1.80	0.63
3:H:144:ASP:HB3	3:H:175:LEU:HD23	1.82	0.60
3:H:29:ILE:HG22	3:H:34:ILE:HD11	1.83	0.60
4:L:105:GLU:HG2	4:L:106:ILE:H	1.66	0.60
1:A:234:TYR:O	1:A:238:ILE:HG13	2.02	0.60
3:H:214:LYS:HB3	3:H:214:LYS:NZ	2.16	0.59
1:A:233:ASN:HB3	4:L:93:ARG:NH2	2.18	0.59
1:A:114:ARG:HB3	1:A:119:GLN:HE22	1.66	0.59
4:L:140:TYR:CD1	4:L:141:PRO:HA	2.39	0.58
3:H:4:LEU:HD23	3:H:102:TYR:CD1	2.40	0.57
4:L:47:LEU:HD22	4:L:58:VAL:CG1	2.34	0.57
4:L:40:PRO:CB	4:L:165:GLU:HG3	2.36	0.56
4:L:45:LYS:HE3	6:L:241:HOH:O	2.06	0.56
1:A:87:LYS:HB2	3:H:54:GLY:O	2.06	0.55
4:L:81:GLU:C	4:L:83:PHE:H	2.08	0.55
4:L:24:ARG:HG2	4:L:70:ASP:OD1	2.07	0.55
4:L:47:LEU:HA	4:L:58:VAL:HG21	1.88	0.55
3:H:82:MET:HE2	3:H:82(C):LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.89	0.54
4:L:16:GLY:HA2	4:L:77:SER:OG	2.08	0.53
6:A:277:HOH:O	5:C:1:NAG:O6	2.15	0.53
1:A:81:GLN:HB3	1:A:83:PHE:HE1	1.73	0.53
1:A:180:MET:CE	1:A:215:TRP:HE1	2.21	0.53
3:H:87:THR:O	3:H:88:ALA:HB2	2.09	0.53
3:H:135:THR:HG22	3:H:185:PRO:HA	1.91	0.52
4:L:6:GLN:HB2	4:L:100:GLN:HE22	1.73	0.52
4:L:187:GLU:HA	4:L:211:ARG:NE	2.24	0.52
3:H:210:LYS:HE3	3:H:212:GLU:HB2	1.90	0.52
4:L:198:HIS:O	4:L:201:LEU:HB2	2.10	0.52
4:L:149:LYS:HA	4:L:153:ALA:O	2.10	0.51
4:L:134:CYS:HB2	4:L:148:TRP:CZ2	2.46	0.51
4:L:11:LEU:C	4:L:11:LEU:HD12	2.32	0.50
3:H:4:LEU:HD23	3:H:102:TYR:HD1	1.76	0.50
4:L:135:LEU:HD11	4:L:137:ASN:HB2	1.94	0.50
4:L:24:ARG:HA	4:L:69:THR:O	2.11	0.50
3:H:6:GLU:HA	3:H:21:SER:O	2.11	0.49
1:A:114:ARG:HB3	1:A:119:GLN:NE2	2.26	0.49
4:L:40:PRO:HB3	4:L:165:GLU:HG3	1.93	0.49
3:H:82:MET:HB3	3:H:82(C):LEU:HD21	1.94	0.49
1:A:60(A):HIS:H	1:A:60(A):HIS:CD2	2.30	0.49
4:L:6:GLN:OE1	4:L:99:GLY:HA3	2.13	0.48
4:L:66:GLY:HA3	4:L:71:PHE:HA	1.95	0.48
1:A:162:LEU:HB3	6:A:301:HOH:O	2.14	0.48
4:L:86:TYR:O	4:L:101:GLY:HA2	2.13	0.48
4:L:39:LYS:HG2	6:L:251:HOH:O	2.14	0.48
3:H:103:TRP:N	3:H:103:TRP:CD1	2.82	0.48
3:H:195:ILE:N	3:H:195:ILE:HD12	2.29	0.47
1:A:180:MET:HE3	1:A:215:TRP:HE1	1.79	0.47
4:L:124:GLN:HE22	4:L:131:SER:N	2.12	0.47
1:A:142:GLY:HA2	1:A:193:GLY:HA3	1.95	0.47
3:H:214:LYS:HZ3	3:H:214:LYS:HB3	1.78	0.47
4:L:167:ASP:HB3	4:L:172:THR:H	1.80	0.47
3:H:116:THR:HA	3:H:146:PHE:O	2.15	0.47
1:A:177:SER:HB2	1:A:178:PRO:HD2	1.95	0.47
4:L:17:ASP:O	4:L:77:SER:HA	2.15	0.47
1:A:171:VAL:HG22	1:A:185:PHE:HE2	1.79	0.46
1:A:49:THR:O	1:A:111(D):CYS:HB2	2.16	0.46
4:L:107:LYS:HA	4:L:140:TYR:OH	2.15	0.46
4:L:124:GLN:HE22	4:L:131:SER:CB	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:212:GLU:HG2	3:H:213:PRO:HD2	1.96	0.46
1:A:86:GLU:O	1:A:87:LYS:HB3	2.17	0.45
1:A:203:LYS:O	1:A:204:ASN:HB2	2.16	0.45
4:L:8:PRO:CG	4:L:11:LEU:HD23	2.46	0.45
1:A:230:ARG:HD2	1:A:233:ASN:HD21	1.80	0.45
3:H:171:GLN:C	3:H:173:SER:H	2.20	0.45
1:A:51:TRP:CD1	1:A:242:ILE:HG23	2.52	0.45
3:H:2:VAL:O	3:H:3:GLN:HG2	2.16	0.45
4:L:83:PHE:O	4:L:84:ALA:HB2	2.17	0.45
4:L:175:LEU:C	4:L:175:LEU:HD23	2.37	0.45
4:L:81:GLU:C	4:L:83:PHE:N	2.70	0.45
3:H:32:THR:OG1	3:H:33:TYR:N	2.50	0.45
1:A:77:THR:OG1	1:A:80:THR:HG23	2.17	0.44
3:H:184:VAL:HB	3:H:185:PRO:HD2	1.99	0.44
1:A:185:PHE:O	1:A:223:HIS:HA	2.18	0.44
4:L:14:SER:O	4:L:17:ASP:HB2	2.18	0.44
1:A:180:MET:HE2	1:A:227:VAL:HG11	1.99	0.44
4:L:21:ILE:HD13	4:L:102:THR:HB	1.99	0.44
4:L:30:SER:HB3	4:L:31:THR:H	1.58	0.44
3:H:27:PHE:HE2	3:H:32:THR:HG21	1.82	0.43
1:A:97:PHE:HB2	3:H:97:ALA:O	2.18	0.43
1:A:181:LEU:C	1:A:181:LEU:HD12	2.38	0.43
4:L:193:ALA:HB2	4:L:208:SER:HB3	2.00	0.43
1:A:190:ALA:O	1:A:219:CYS:HB3	2.19	0.42
4:L:113:PRO:HB3	4:L:139:PHE:HB3	2.01	0.42
3:H:95:TRP:HA	6:H:230:HOH:O	2.19	0.42
4:L:181:LEU:N	4:L:181:LEU:HD12	2.35	0.42
4:L:121:SER:OG	4:L:124:GLN:HB2	2.19	0.42
4:L:124:GLN:HE22	4:L:131:SER:H	1.68	0.42
3:H:195:ILE:HA	3:H:209:LYS:O	2.19	0.42
3:H:195:ILE:HG23	3:H:209:LYS:O	2.19	0.42
4:L:6:GLN:HG2	4:L:88:CYS:SG	2.59	0.42
4:L:154:LEU:HD13	4:L:154:LEU:C	2.40	0.42
4:L:55:TYR:O	4:L:56:SER:C	2.58	0.42
1:A:48:HIS:CE1	1:A:49:THR:HG23	2.55	0.41
1:A:98:ASN:ND2	1:A:100:ASP:HB2	2.35	0.41
1:A:67:VAL:CG1	1:A:70:GLN:HE21	2.32	0.41
4:L:54:LEU:HD11	4:L:58:VAL:CG1	2.50	0.41
3:H:173:SER:O	3:H:175:LEU:HD13	2.19	0.41
1:A:71:HIS:CE1	1:A:154:SER:HB2	2.56	0.41
3:H:95:TRP:CD1	3:H:95:TRP:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:138:ASN:HA	4:L:173:TYR:O	2.21	0.41
4:L:139:PHE:CD1	4:L:139:PHE:N	2.89	0.41
1:A:235:VAL:HG12	1:A:239:ASN:ND2	2.35	0.41
1:A:122:CYS:SG	2:B:393:CYS:C	2.99	0.41
3:H:212:GLU:HG2	3:H:213:PRO:CD	2.50	0.41
3:H:95:TRP:O	3:H:96:TRP:HB2	2.20	0.41
4:L:40:PRO:HG2	4:L:83:PHE:CE2	2.56	0.41
4:L:201:LEU:HG	4:L:205:VAL:HG23	2.03	0.41
4:L:136:LEU:HD13	4:L:175:LEU:HD22	2.02	0.40
1:A:222:LEU:O	1:A:223:HIS:HB2	2.22	0.40
1:A:180:MET:CE	1:A:227:VAL:HG11	2.52	0.40
3:H:166:PHE:HA	3:H:167:PRO:HD3	1.87	0.40
1:A:195:SER:HB2	6:A:37:HOH:O	2.21	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	225/257 (88%)	204 (91%)	21 (9%)	0	100	100
2	B	3/35 (9%)	3 (100%)	0	0	100	100
3	H	211/225 (94%)	194 (92%)	15 (7%)	2 (1%)	17	17
4	L	202/214 (94%)	181 (90%)	17 (8%)	4 (2%)	7	5
All	All	641/731 (88%)	582 (91%)	53 (8%)	6 (1%)	17	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	96	TRP
3	H	144	ASP

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Mol	Chain	Res	Type
4	L	17	ASP
4	L	138	ASN
4	L	204	PRO
4	L	82	ASP

### 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	195/213 (92%)	188 (96%)	7 (4%)	35	43
2	B	3/30 (10%)	2 (67%)	1 (33%)	0	0
3	H	173/182 (95%)	168 (97%)	5 (3%)	42	52
4	L	181/186 (97%)	174 (96%)	7 (4%)	32	40
All	All	552/611 (90%)	532 (96%)	20 (4%)	35	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	57	HIS
1	A	111(B)	ASP
1	A	145	ASP
1	A	160	VAL
1	A	170(B)	GLU
1	A	195	SER
2	B	395	ARG
3	H	94	LYS
3	H	95	TRP
3	H	138	LEU
3	H	149	PRO
3	H	199	ASN
4	L	17	ASP
4	L	30	SER
4	L	83	PHE
4	L	137	ASN

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Mol	Chain	Res	Type
4	L	147	GLN
4	L	174	SER
4	L	181	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	60(A)	HIS
1	A	70	GLN
1	A	119	GLN
1	A	143	HIS
1	A	192	GLN
1	A	204	ASN
1	A	233	ASN
3	H	13	GLN
3	H	30	ASN
3	H	199	ASN
4	L	3	GLN
4	L	92	ASN
4	L	124	GLN
4	L	137	ASN
4	L	147	GLN
4	L	189	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 monosaccharides 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
5	NAG	C	1	1,5	14,14,15	0.57	0	17,19,21	0.99	1 (5%)
5	NAG	C	2	5	14,14,15	0.50	0	17,19,21	2.19	4 (23%)

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	NAG	C	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	NAG	C4-C3-C2	-5.99	102.23	111.02
5	C	2	NAG	C1-O5-C5	4.09	117.73	112.19
5	C	2	NAG	C2-N2-C7	-2.76	118.98	122.90
5	C	2	NAG	O4-C4-C5	2.45	115.39	109.30
5	C	1	NAG	O5-C1-C2	-2.31	107.64	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	2	0



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	233/257 (90%)	0.98	45 (19%) 1 2	37, 63, 93, 106	1 (0%)
2	B	5/35 (14%)	1.41	2 (40%) 0 0	74, 78, 84, 89	0
3	H	215/225 (95%)	0.70	28 (13%) 3 5	30, 62, 98, 119	1 (0%)
4	L	208/214 (97%)	0.85	27 (12%) 3 5	40, 75, 86, 110	0
All	All	661/731 (90%)	0.85	102 (15%) 2 3	30, 68, 92, 119	2 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	216	CYS	10.8
4	L	214	CYS	8.2
1	A	222	LEU	6.9
3	H	69	ILE	6.4
1	A	187	CYS	6.0
1	A	148	VAL	5.8
3	H	190	GLY	5.3
3	H	135	THR	4.7
1	A	223	HIS	4.6
4	L	34	ALA	4.6
3	H	139	GLY	4.5
1	A	144	LEU	4.2
1	A	143	HIS	4.1
3	H	215	SER	4.1
2	B	392	ALA	4.1
1	A	192	GLN	3.9
1	A	145	ASP	3.8
1	A	79	VAL	3.8
3	H	140	CYS	3.5
1	A	31	ALA	3.4
1	A	106	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
3	H	124	LEU	3.4
3	H	141	LEU	3.4
1	A	105	LEU	3.4
2	B	395	ARG	3.2
4	L	35	TRP	3.2
4	L	88	CYS	3.2
1	A	111(B)	ASP	3.2
3	H	214	LYS	3.2
4	L	33	VAL	3.2
1	A	111(C)	ARG	3.2
4	L	26	SER	3.2
3	H	90	TYR	3.1
1	A	185	PHE	3.1
1	A	200	ALA	3.1
1	A	23	LEU	3.1
4	L	104	VAL	3.0
4	L	36	TYR	3.0
1	A	182	CYS	3.0
1	A	53	VAL	3.0
1	A	18	GLY	2.9
4	L	183	LYS	2.9
4	L	77	SER	2.9
1	A	205	GLY	2.9
1	A	29	TRP	2.9
3	H	173	SER	2.9
1	A	199	LEU	2.9
4	L	86	TYR	2.9
4	L	171	SER	2.8
3	H	136	ALA	2.8
3	H	109	VAL	2.8
1	A	44	GLY	2.8
1	A	138	ILE	2.8
1	A	114	ARG	2.7
3	H	138	LEU	2.7
1	A	175	ASP	2.7
1	A	243	ARG	2.6
1	A	215	TRP	2.6
4	L	213	GLU	2.6
4	L	154	LEU	2.5
4	L	166	GLN	2.5
1	A	183	ALA	2.5
3	H	92	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
4	L	175	LEU	2.5
1	A	16	ILE	2.4
1	A	170(B)	GLU	2.4
3	H	33	TYR	2.4
3	H	186	SER	2.4
1	A	90	PRO	2.4
4	L	91	SER	2.4
3	H	80	LEU	2.3
4	L	24	ARG	2.3
1	A	52	VAL	2.3
3	H	41	PRO	2.3
3	H	213	PRO	2.3
3	H	34	ILE	2.3
4	L	18	ARG	2.3
1	A	162	LEU	2.2
1	A	107	ARG	2.2
1	A	30	LEU	2.2
4	L	32	ALA	2.2
4	L	108	ARG	2.2
1	A	45	SER	2.2
3	H	115	SER	2.2
4	L	156	SER	2.2
3	H	43	LYS	2.2
1	A	91	TYR	2.2
3	H	180	SER	2.2
3	H	181	VAL	2.2
4	L	212	GLY	2.2
4	L	107	LYS	2.1
1	A	170	SER	2.1
1	A	163	VAL	2.1
4	L	14	SER	2.1
1	A	92	THR	2.1
1	A	117	PHE	2.1
1	A	32	ALA	2.1
4	L	173	TYR	2.1
1	A	203	LYS	2.0
3	H	188	SER	2.0
4	L	23	CYS	2.0
3	H	195	ILE	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	2	14/15	0.75	0.49	71,75,84,84	0
5	NAG	C	1	14/15	0.78	0.18	53,64,68,68	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.