



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 03:25 PM EST

PDB ID : 6VY4  
Title : Crystal structure of Hendra receptor binding protein head domain in complex with human neutralizing antibody HENV-32  
Authors : Dong, J.; Crowe, J.E.  
Deposited on : 2020-02-25  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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:

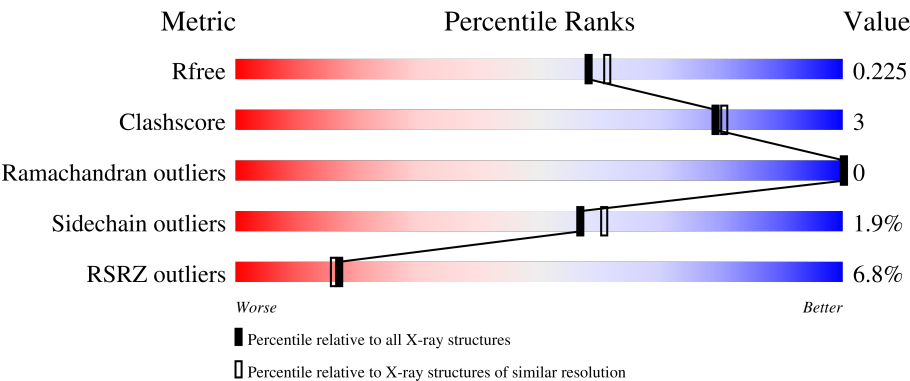
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	433	<div><div>0%</div><div>90%</div><div>7%</div><div>••</div></div>
1	B	433	<div><div>3%</div><div>93%</div><div>5%</div><div>•</div></div>
2	C	221	<div><div>5%</div><div>84%</div><div>10%</div><div>6%</div></div>
2	H	221	<div><div>6%</div><div>89%</div><div>7%</div><div>5%</div></div>
3	D	214	<div><div>26%</div><div>86%</div><div>6%</div><div>• 7%</div></div>

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Mol	Chain	Length	Quality of chain
3	L	214	 8%87%11%

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
4	SO4	A	701	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13613 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 receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	1	0
			3317	2116	559	623	19			
1	B	426	Total	C	N	O	S	0	2	0
			3343	2135	561	628	19			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	GLU	-	expression tag	UNP F4YH71
A	606	ASN	-	expression tag	UNP F4YH71
A	607	LEU	-	expression tag	UNP F4YH71
A	608	TYR	-	expression tag	UNP F4YH71
A	609	PHE	-	expression tag	UNP F4YH71
A	610	GLN	-	expression tag	UNP F4YH71
A	611	GLY	-	expression tag	UNP F4YH71
A	612	HIS	-	expression tag	UNP F4YH71
A	613	HIS	-	expression tag	UNP F4YH71
A	614	HIS	-	expression tag	UNP F4YH71
A	615	HIS	-	expression tag	UNP F4YH71
A	616	HIS	-	expression tag	UNP F4YH71
A	617	HIS	-	expression tag	UNP F4YH71
B	605	GLU	-	expression tag	UNP F4YH71
B	606	ASN	-	expression tag	UNP F4YH71
B	607	LEU	-	expression tag	UNP F4YH71
B	608	TYR	-	expression tag	UNP F4YH71
B	609	PHE	-	expression tag	UNP F4YH71
B	610	GLN	-	expression tag	UNP F4YH71
B	611	GLY	-	expression tag	UNP F4YH71
B	612	HIS	-	expression tag	UNP F4YH71
B	613	HIS	-	expression tag	UNP F4YH71
B	614	HIS	-	expression tag	UNP F4YH71
B	615	HIS	-	expression tag	UNP F4YH71
B	616	HIS	-	expression tag	UNP F4YH71

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Chain	Residue	Modelled	Actual	Comment	Reference
B	617	HIS	-	expression tag	UNP F4YH71

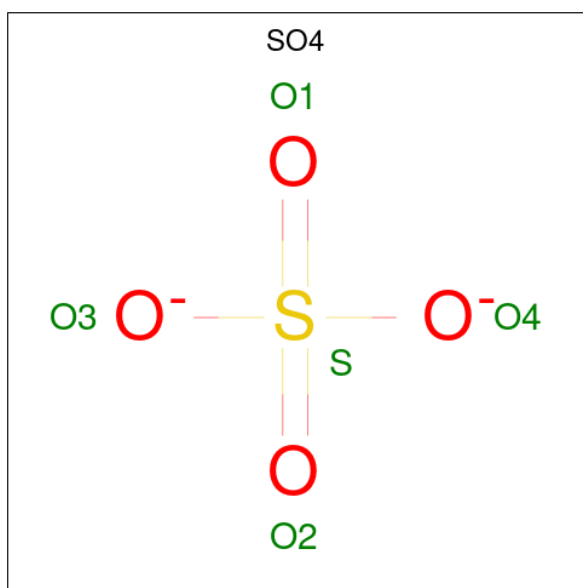
- Molecule 2 is a protein called Anti-Hendra receptor binding protein antibody HENV-32 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1555	990	269	290	6			
2	H	211	Total	C	N	O	S	0	0	0
			1582	1007	269	300	6			

- Molecule 3 is a protein called Anti-Hendra receptor binding protein antibody HENV-32 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	198	Total	C	N	O	S	0	0	0
			1389	861	242	282	4			
3	L	210	Total	C	N	O	S	0	0	0
			1543	961	264	314	4			

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



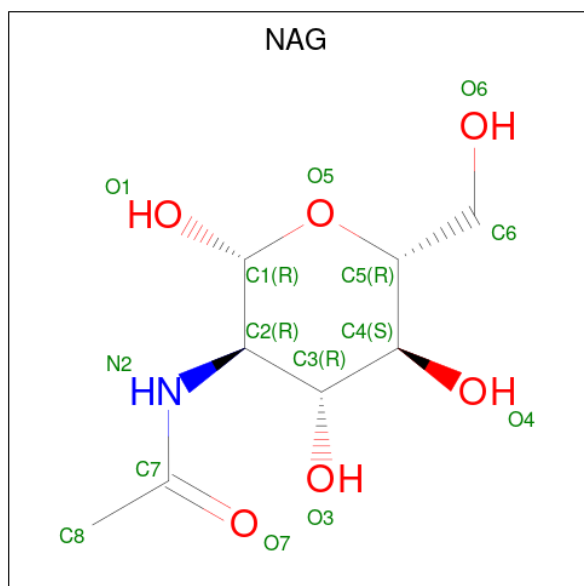
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



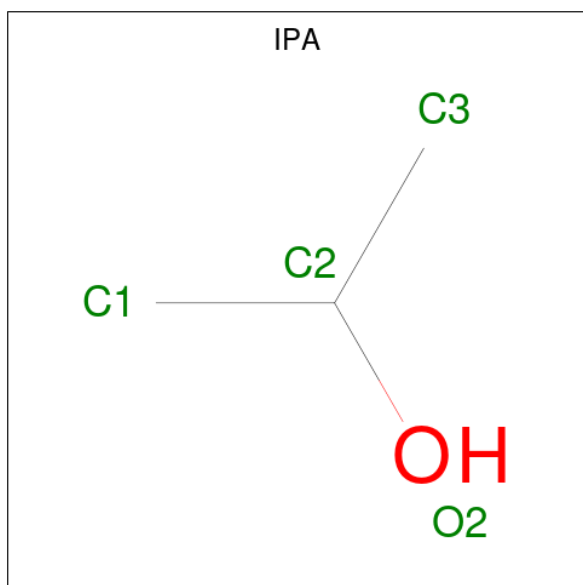
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	315	Total	O	0	0
			315	315		
7	B	242	Total	O	0	0
			242	242		
7	C	50	Total	O	0	0
			50	50		
7	D	37	Total	O	0	0
			37	37		

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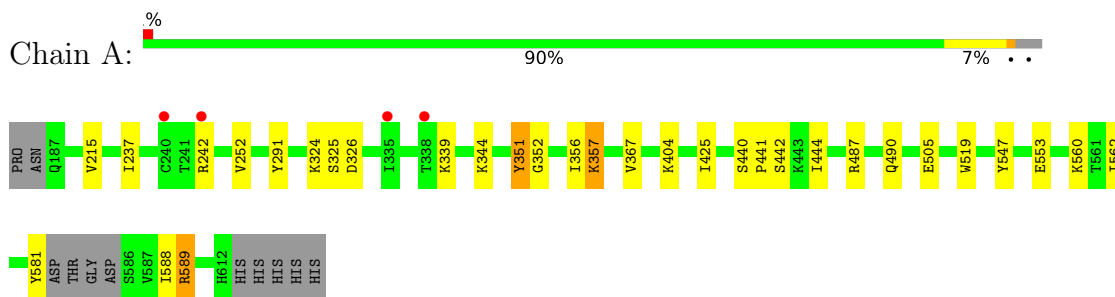
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	33	Total 33	O 33	0	0
7	L	44	Total 44	O 44	0	0



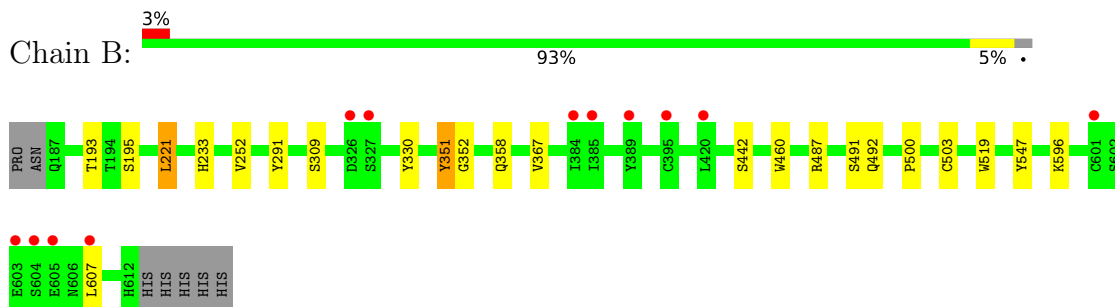
### 3 Residue-property plots [i](#)

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.

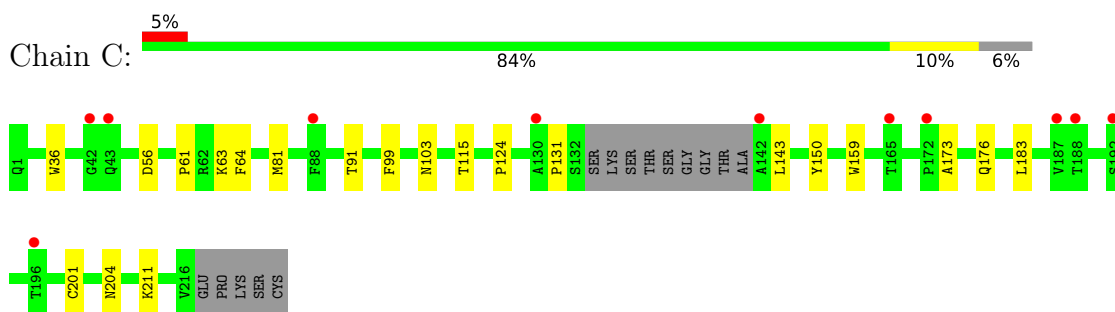
- Molecule 1: receptor binding protein



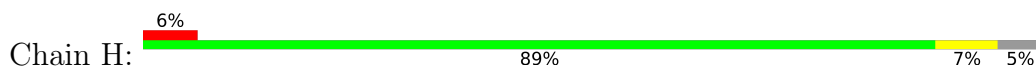
- Molecule 1: receptor binding protein

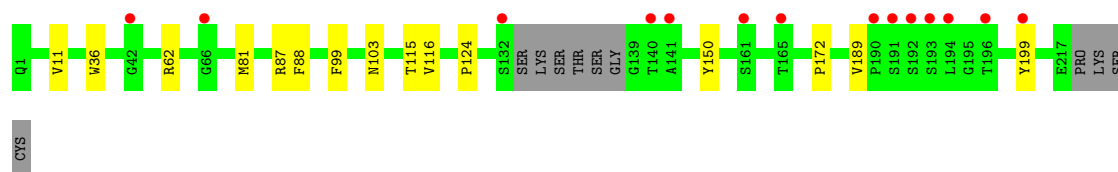


- Molecule 2: Anti-Hendra receptor binding protein antibody HENV-32 Fab heavy chain

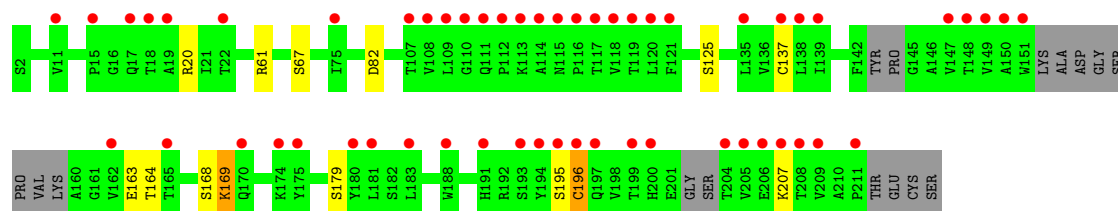
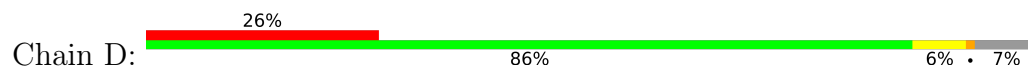


- Molecule 2: Anti-Hendra receptor binding protein antibody HENV-32 Fab heavy chain

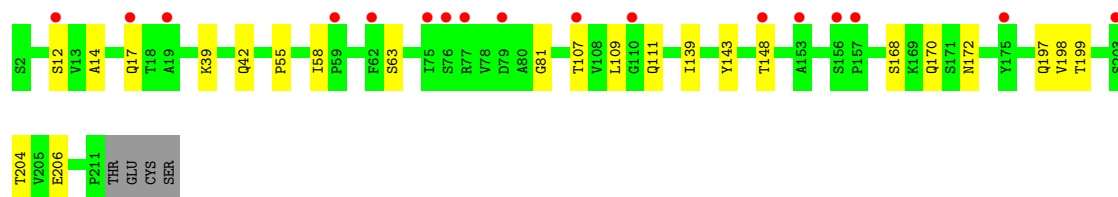
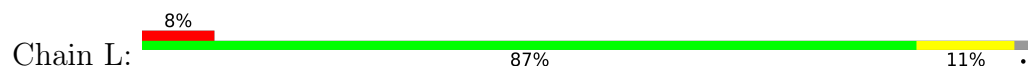




- Molecule 3: Anti-Hendra receptor binding protein antibody HENV-32 Fab light chain



- Molecule 3: Anti-Hendra receptor binding protein antibody HENV-32 Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.89Å 84.49Å 122.83Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	49.51 – 2.00 49.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.51-2.00) 100.0 (49.50-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.183 , 0.226 0.183 , 0.225	Depositor DCC
$R_{free}$ test set	6714 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13613	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: IPA, NAG, SO4

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	0.48	0/3397	0.61	0/4627
1	B	0.51	1/3431 (0.0%)	0.60	0/4676
2	C	0.39	0/1595	0.55	0/2172
2	H	0.40	0/1622	0.53	0/2212
3	D	0.33	0/1417	0.54	1/1942 (0.1%)
3	L	0.33	0/1582	0.51	0/2169
All	All	0.44	1/13044 (0.0%)	0.57	1/17798 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	503	CYS	CB-SG	-7.23	1.70	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	196	CYS	CA-CB-SG	10.13	132.24	114.00

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	3317	0	3228	19	0
1	B	3343	0	3246	13	0
2	C	1555	0	1501	10	0
2	H	1582	0	1545	8	0
3	D	1389	0	1231	8	0
3	L	1543	0	1438	13	0
4	A	5	0	0	1	1
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	H	5	0	0	0	0
5	A	56	0	52	0	0
5	B	70	0	65	2	0
6	A	8	0	16	0	0
6	B	4	0	8	0	0
7	A	315	0	0	6	1
7	B	242	0	0	2	1
7	C	50	0	0	1	0
7	D	37	0	0	0	0
7	H	33	0	0	0	0
7	L	44	0	0	0	0
All	All	13613	0	12330	70	2

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 3.

All (70) 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:581:TYR:HB2	1:A:588:ILE:HG12	1.59	0.83
3:D:137:CYS:CB	3:D:196:CYS:HG	2.02	0.73
1:A:344:LYS:NZ	7:A:802:HOH:O	2.24	0.70
1:B:596:LYS:NZ	7:B:802:HOH:O	2.26	0.68
2:C:91:THR:HG23	2:C:115:THR:HA	1.77	0.67
3:D:164:THR:HG23	3:D:179:SER:HB2	1.77	0.67
1:B:221:LEU:C	1:B:221:LEU:HD23	2.16	0.65
2:H:87:ARG:O	2:H:116:VAL:HG21	1.97	0.63
5:B:707:NAG:H3	5:B:707:NAG:H83	1.80	0.62
3:D:137:CYS:HG	3:D:196:CYS:CB	2.11	0.61
3:D:137:CYS:SG	3:D:196:CYS:CB	2.90	0.59
4:A:701:SO4:O2	7:A:801:HOH:O	2.11	0.59
1:A:215:VAL:HG22	1:A:237:ILE:HD13	1.85	0.58
3:L:39:LYS:NZ	3:L:81:GLY:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:12:SER:HB2	3:L:109:LEU:HD13	1.85	0.57
3:L:14:ALA:HB3	3:L:17:GLN:NE2	2.20	0.57
3:L:199:THR:HG22	3:L:204:THR:OG1	2.05	0.56
1:A:589:ARG:NH2	1:A:589:ARG:HB2	2.21	0.55
1:B:193:THR:HG22	1:B:195:SER:H	1.72	0.54
2:C:124:PRO:HB3	2:C:150:TYR:HB3	1.89	0.53
2:C:63:LYS:HG2	7:C:416:HOH:O	2.08	0.52
2:H:88:PHE:HA	2:H:116:VAL:CG2	2.40	0.52
3:L:148:THR:OG1	3:L:199:THR:OG1	2.27	0.52
1:A:351:TYR:HD2	1:A:367:VAL:HB	1.75	0.51
1:A:357:LYS:NZ	7:A:811:HOH:O	2.44	0.50
1:A:404:LYS:NZ	7:A:810:HOH:O	2.44	0.49
1:A:339:LYS:HG3	1:A:425:ILE:HG23	1.93	0.49
3:L:111:GLN:HB2	3:L:143:TYR:CZ	2.48	0.49
2:C:173:ALA:HA	2:C:183:LEU:HB3	1.95	0.48
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.96	0.47
2:H:189:VAL:HG21	2:H:199:TYR:CZ	2.49	0.47
1:A:242:ARG:HD3	1:B:330:TYR:HD1	1.80	0.47
3:D:61:ARG:NH1	3:D:82:ASP:OD2	2.48	0.47
1:B:491:SER:HB2	1:B:492:GLN:HE21	1.80	0.47
1:A:560:LYS:HE2	1:A:562:ILE:HD11	1.96	0.46
1:B:252:VAL:HG11	1:B:291:TYR:HB2	1.98	0.46
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.50	0.46
1:B:351:TYR:HD2	1:B:367:VAL:HB	1.80	0.46
1:A:440:SER:HB2	1:A:441:PRO:HD2	1.98	0.45
1:A:490:GLN:HB2	1:A:505:GLU:CD	2.37	0.45
1:A:344:LYS:HG2	7:A:806:HOH:O	2.17	0.45
1:B:221:LEU:C	1:B:221:LEU:CD2	2.84	0.44
3:L:55:PRO:HD2	3:L:58:ILE:HG13	1.99	0.44
1:A:252:VAL:HG11	1:A:291:TYR:HB2	1.98	0.44
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.53	0.44
1:B:460:TRP:CD2	1:B:500:PRO:HA	2.52	0.44
1:B:351:TYR:CD2	1:B:367:VAL:HB	2.53	0.44
2:C:131:PRO:HD3	2:C:143:LEU:HB3	1.99	0.44
1:A:490:GLN:HG2	1:B:358:GLN:HB3	1.99	0.43
2:C:204:ASN:HD21	2:C:211:LYS:CE	2.31	0.43
2:H:88:PHE:HA	2:H:116:VAL:HG23	2.00	0.43
1:A:324:LYS:NZ	7:A:803:HOH:O	2.27	0.43
5:B:705:NAG:H83	7:B:886:HOH:O	2.18	0.43
2:C:61:PRO:HG2	2:C:64:PHE:HD2	1.84	0.43
2:H:172:PRO:HG2	3:L:168:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:GLU:OE1	1:A:553:GLU:N	2.52	0.43
1:B:352:GLY:HA3	1:B:442:SER:O	2.19	0.42
1:B:607:LEU:H	1:B:607:LEU:HD12	1.85	0.42
2:C:159:TRP:CH2	2:C:201:CYS:HB3	2.55	0.42
3:L:139:ILE:HG12	3:L:198:VAL:HG21	2.01	0.42
3:D:168:SER:OG	3:D:169:LYS:N	2.52	0.41
1:A:352:GLY:HA3	1:A:442:SER:O	2.20	0.41
2:H:11:VAL:HA	2:H:115:THR:O	2.21	0.41
3:L:42:GLN:HG2	3:L:42:GLN:H	1.65	0.41
2:C:176:GLN:HA	3:D:163:GLU:OE2	2.21	0.41
3:L:12:SER:HA	3:L:107:THR:O	2.20	0.41
3:D:195:SER:HA	3:D:207:LYS:O	2.21	0.40
1:A:356:ILE:HG12	1:A:444:ILE:HG12	2.03	0.40
3:L:170:GLN:HB2	3:L:172:ASN:OD1	2.20	0.40
3:L:197:GLN:NE2	3:L:206:GLU:OE2	2.52	0.40

All (2) 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)
4:A:701:SO4:O4	7:A:801:HOH:O[2_556]	2.13	0.07
7:B:1041:HOH:O	7:B:1041:HOH:O[2_556]	2.15	0.05

## 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	419/433 (97%)	403 (96%)	16 (4%)	0	100	100
1	B	426/433 (98%)	410 (96%)	16 (4%)	0	100	100
2	C	203/221 (92%)	199 (98%)	4 (2%)	0	100	100
2	H	207/221 (94%)	202 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	190/214 (89%)	185 (97%)	5 (3%)	0	100	100
3	L	208/214 (97%)	204 (98%)	4 (2%)	0	100	100
All	All	1653/1736 (95%)	1603 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	370/389 (95%)	362 (98%)	8 (2%)	52	55
1	B	371/389 (95%)	364 (98%)	7 (2%)	57	61
2	C	167/190 (88%)	164 (98%)	3 (2%)	59	63
2	H	175/190 (92%)	172 (98%)	3 (2%)	60	65
3	D	134/178 (75%)	130 (97%)	4 (3%)	41	41
3	L	165/178 (93%)	164 (99%)	1 (1%)	86	90
All	All	1382/1514 (91%)	1356 (98%)	26 (2%)	57	61

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

Mol	Chain	Res	Type
1	A	325	SER
1	A	326	ASP
1	A	351	TYR
1	A	357	LYS
1	A	487	ARG
1	A	519	TRP
1	A	547	TYR
1	A	589	ARG
1	B	221	LEU
1	B	233	HIS
1	B	309	SER
1	B	351	TYR

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Mol	Chain	Res	Type
1	B	487	ARG
1	B	519	TRP
1	B	547	TYR
2	C	56	ASP
2	C	99	PHE
2	C	103	ASN
3	D	20	ARG
3	D	67	SER
3	D	125	SER
3	D	169	LYS
2	H	62	ARG
2	H	99	PHE
2	H	103	ASN
3	L	63	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	492	GLN
2	C	169	HIS
2	C	204	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

17 ligands 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	A	705	1	14,14,15	0.59	0	17,19,21	0.39	0
4	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.20	0
5	NAG	B	704	1	14,14,15	0.29	0	17,19,21	0.53	0
4	SO4	B	701	-	4,4,4	0.17	0	6,6,6	0.31	0
5	NAG	B	703	1	14,14,15	0.17	0	17,19,21	0.46	0
5	NAG	A	703	1	14,14,15	0.56	0	17,19,21	0.51	0
4	SO4	B	702	-	4,4,4	0.12	0	6,6,6	0.25	0
5	NAG	B	707	1	14,14,15	0.68	1 (7%)	17,19,21	1.20	1 (5%)
4	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.27	0
6	IPA	A	706	-	3,3,3	0.57	0	3,3,3	0.25	0
4	SO4	A	701	-	4,4,4	0.17	0	6,6,6	0.62	0
5	NAG	A	704	1	14,14,15	0.34	0	17,19,21	0.53	0
6	IPA	A	707	-	3,3,3	0.53	0	3,3,3	0.55	0
5	NAG	B	708	1	14,14,15	0.26	0	17,19,21	0.88	1 (5%)
5	NAG	B	705	1	14,14,15	0.46	0	17,19,21	0.45	0
5	NAG	A	702	1	14,14,15	0.39	0	17,19,21	0.53	0
6	IPA	B	706	-	3,3,3	0.49	0	3,3,3	0.48	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	NAG	B	704	1	-	0/6/23/26	0/1/1/1
5	NAG	B	703	1	-	0/6/23/26	0/1/1/1
5	NAG	A	703	1	-	0/6/23/26	0/1/1/1
5	NAG	B	707	1	-	3/6/23/26	0/1/1/1
5	NAG	A	704	1	-	0/6/23/26	0/1/1/1
5	NAG	A	705	1	-	0/6/23/26	0/1/1/1
5	NAG	B	708	1	-	3/6/23/26	0/1/1/1
5	NAG	B	705	1	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	707	NAG	C1-C2	2.23	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	707	NAG	C2-N2-C7	4.18	128.86	122.90
5	B	708	NAG	C1-O5-C5	2.42	115.47	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	707	NAG	C8-C7-N2-C2
5	B	707	NAG	O7-C7-N2-C2
5	B	705	NAG	C8-C7-N2-C2
5	B	705	NAG	O7-C7-N2-C2
5	B	708	NAG	O5-C5-C6-O6
5	B	708	NAG	C4-C5-C6-O6
5	B	708	NAG	C3-C2-N2-C7
5	B	707	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	707	NAG	1	0
4	A	701	SO4	1	1
5	B	705	NAG	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	422/433 (97%)	-0.03	4 (0%) 84 83	22, 34, 64, 89	0
1	B	426/433 (98%)	0.31	12 (2%) 53 51	21, 35, 72, 124	0
2	C	207/221 (93%)	0.14	11 (5%) 26 25	27, 56, 102, 119	0
2	H	211/221 (95%)	0.16	14 (6%) 18 17	31, 54, 91, 104	0
3	D	198/214 (92%)	1.28	55 (27%) 0 0	32, 74, 108, 121	0
3	L	210/214 (98%)	0.45	17 (8%) 12 11	31, 61, 84, 100	0
All	All	1674/1736 (96%)	0.32	113 (6%) 17 16	21, 46, 91, 124	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	604	SER	8.0
3	D	150	ALA	7.6
3	D	205	VAL	6.4
3	D	204	THR	6.3
3	D	147	VAL	6.0
3	D	209	VAL	5.6
3	D	114	ALA	5.4
3	D	208	THR	5.1
1	B	389	TYR	5.1
3	D	118	VAL	4.9
3	D	194	TYR	4.7
2	H	194	LEU	4.6
3	D	196	CYS	4.5
3	D	115	ASN	4.4
2	C	130	ALA	4.3
3	D	197	GLN	4.0
3	D	149	VAL	4.0
3	D	116	PRO	3.9
3	D	139	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	199	THR	3.8
2	C	192	SER	3.7
2	H	199	TYR	3.7
3	D	200	HIS	3.6
3	D	181	LEU	3.6
3	D	175	TYR	3.6
1	B	327	SER	3.5
3	D	109	LEU	3.5
3	D	183	LEU	3.4
2	H	66	GLY	3.4
3	D	148	THR	3.3
3	D	195	SER	3.3
2	C	187	VAL	3.3
3	D	11	VAL	3.3
3	L	76	SER	3.2
1	B	603	GLU	3.2
2	H	196	THR	3.2
1	B	326	ASP	3.2
3	D	120	LEU	3.2
3	D	193	SER	3.1
3	D	111	GLN	3.1
1	B	607	LEU	3.0
3	D	188	TRP	3.0
2	H	132	SER	3.0
3	D	137	CYS	3.0
1	B	385	ILE	3.0
1	A	335	ILE	2.9
1	B	420	LEU	2.9
2	H	161	SER	2.9
2	H	190	PRO	2.9
3	L	153	ALA	2.9
1	B	605	GLU	2.9
2	H	141	ALA	2.9
2	H	192	SER	2.8
2	C	196	THR	2.8
3	D	119	THR	2.8
2	H	42	GLY	2.7
3	D	151	TRP	2.7
3	D	191	HIS	2.7
3	D	170	GLN	2.7
3	D	206	GLU	2.7
2	H	193	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	162	VAL	2.6
3	D	117	THR	2.6
3	L	79	ASP	2.6
3	D	207	LYS	2.6
3	L	19	ALA	2.6
3	D	22	THR	2.6
1	B	395	CYS	2.6
3	L	157	PRO	2.6
3	D	113	LYS	2.5
2	H	140	THR	2.5
3	L	12	SER	2.5
2	C	188	THR	2.5
3	L	75	ILE	2.5
3	L	17	GLN	2.5
3	L	156	SER	2.5
1	B	601	CYS	2.5
1	A	240	CYS	2.4
3	D	211	PRO	2.4
3	D	135	LEU	2.4
3	D	180	TYR	2.4
3	D	165	THR	2.4
3	D	110	GLY	2.4
3	D	121	PHE	2.4
2	C	42	GLY	2.4
3	D	107	THR	2.3
3	L	148	THR	2.3
3	L	203	SER	2.3
1	A	338	THR	2.3
3	D	18	THR	2.3
2	C	172	PRO	2.3
3	D	17	GLN	2.3
2	H	191	SER	2.2
3	D	75	ILE	2.2
2	C	43	GLN	2.2
3	L	77	ARG	2.2
3	D	15	PRO	2.2
3	D	19	ALA	2.2
1	A	242	ARG	2.2
3	L	107	THR	2.1
1	B	384	ILE	2.1
3	D	108	VAL	2.1
3	D	112	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	59	PRO	2.1
2	H	165	THR	2.1
3	D	174	LYS	2.1
3	L	110	GLY	2.1
2	C	165	THR	2.1
2	C	88	PHE	2.1
3	L	62	PHE	2.0
3	D	138	LEU	2.0
2	C	142	ALA	2.0
3	L	175	TYR	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](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
5	NAG	B	708	14/15	0.64	0.29	95,102,111,115	0
5	NAG	B	703	14/15	0.79	0.17	70,77,81,81	0
6	IPA	A	706	4/4	0.81	0.13	63,66,69,70	0
5	NAG	B	707	14/15	0.81	0.18	67,79,101,105	0
5	NAG	B	705	14/15	0.86	0.18	49,59,74,74	0
6	IPA	A	707	4/4	0.90	0.25	53,55,55,55	0
5	NAG	A	702	14/15	0.90	0.14	51,58,64,68	0
5	NAG	A	703	14/15	0.92	0.11	30,40,48,52	0
4	SO4	B	702	5/5	0.94	0.13	74,76,77,77	0
6	IPA	B	706	4/4	0.94	0.26	48,56,56,58	0
5	NAG	B	704	14/15	0.95	0.11	32,37,42,44	0
5	NAG	A	705	14/15	0.95	0.11	27,39,43,48	0
5	NAG	A	704	14/15	0.95	0.12	28,33,38,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	H	301	5/5	0.96	0.21	76,76,82,83	0
4	SO4	C	301	5/5	0.96	0.14	57,63,75,75	0
4	SO4	A	701	5/5	0.97	0.19	35,37,45,46	5
4	SO4	B	701	5/5	0.98	0.14	48,55,59,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.