



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:59 PM UTC

PDB ID : 5KOV / pdb\_00005kov  
Title : Crystal structure of the human astrovirus 2 capsid protein spike in complex with a single chain variable fragment of an astrovirus neutralizing antibody at 3.24-Å resolution  
Authors : Bogdanoff, W.A.; DuBois, R.M.  
Deposited on : 2016-07-01  
Resolution : 3.25 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

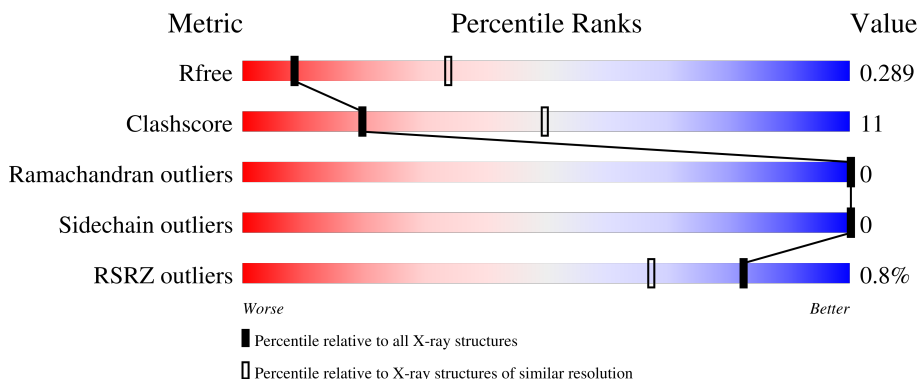
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

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













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	228	
1	B	228	
1	G	228	
1	H	228	
1	M	228	

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Mol	Chain	Length	Quality of chain
1	N	228	 71% 24% 5%
1	S	228	 73% 22% 5%
1	T	228	 69% 25% 5%
2	C	251	 65% 24% 11%
2	E	251	 2% 65% 24% 11%
2	I	251	 2% 70% 20% 10%
2	K	251	 67% 22% 11%
2	O	251	 2% 60% 24% 16%
2	Q	251	 29% 8% 63%
2	U	251	 2% 65% 23% 12%
2	W	251	 30% 12% 58%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25943 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 Capsid polyprotein VP90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0
1	B	218	Total 1756	C 1125	N 292	O 330	S 9	0	0	0
1	H	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0
1	G	219	Total 1760	C 1127	N 293	O 331	S 9	0	0	0
1	N	217	Total 1750	C 1121	N 291	O 329	S 9	0	0	0
1	M	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0
1	S	218	Total 1755	C 1124	N 292	O 330	S 9	0	0	0
1	T	216	Total 1745	C 1118	N 290	O 328	S 9	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	MET	-	initiating methionine	UNP Q82446
A	428	GLY	-	expression tag	UNP Q82446
A	645	ALA	-	expression tag	UNP Q82446
A	646	ALA	-	expression tag	UNP Q82446
A	647	ALA	-	expression tag	UNP Q82446
A	648	GLU	-	expression tag	UNP Q82446
A	649	LEU	-	expression tag	UNP Q82446
A	650	ALA	-	expression tag	UNP Q82446
A	651	LEU	-	expression tag	UNP Q82446
A	652	VAL	-	expression tag	UNP Q82446
A	653	PRO	-	expression tag	UNP Q82446
A	654	ARG	-	expression tag	UNP Q82446
B	427	MET	-	initiating methionine	UNP Q82446

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Chain	Residue	Modelled	Actual	Comment	Reference
B	428	GLY	-	expression tag	UNP Q82446
B	645	ALA	-	expression tag	UNP Q82446
B	646	ALA	-	expression tag	UNP Q82446
B	647	ALA	-	expression tag	UNP Q82446
B	648	GLU	-	expression tag	UNP Q82446
B	649	LEU	-	expression tag	UNP Q82446
B	650	ALA	-	expression tag	UNP Q82446
B	651	LEU	-	expression tag	UNP Q82446
B	652	VAL	-	expression tag	UNP Q82446
B	653	PRO	-	expression tag	UNP Q82446
B	654	ARG	-	expression tag	UNP Q82446
H	427	MET	-	initiating methionine	UNP Q82446
H	428	GLY	-	expression tag	UNP Q82446
H	645	ALA	-	expression tag	UNP Q82446
H	646	ALA	-	expression tag	UNP Q82446
H	647	ALA	-	expression tag	UNP Q82446
H	648	GLU	-	expression tag	UNP Q82446
H	649	LEU	-	expression tag	UNP Q82446
H	650	ALA	-	expression tag	UNP Q82446
H	651	LEU	-	expression tag	UNP Q82446
H	652	VAL	-	expression tag	UNP Q82446
H	653	PRO	-	expression tag	UNP Q82446
H	654	ARG	-	expression tag	UNP Q82446
G	427	MET	-	initiating methionine	UNP Q82446
G	428	GLY	-	expression tag	UNP Q82446
G	645	ALA	-	expression tag	UNP Q82446
G	646	ALA	-	expression tag	UNP Q82446
G	647	ALA	-	expression tag	UNP Q82446
G	648	GLU	-	expression tag	UNP Q82446
G	649	LEU	-	expression tag	UNP Q82446
G	650	ALA	-	expression tag	UNP Q82446
G	651	LEU	-	expression tag	UNP Q82446
G	652	VAL	-	expression tag	UNP Q82446
G	653	PRO	-	expression tag	UNP Q82446
G	654	ARG	-	expression tag	UNP Q82446
N	427	MET	-	initiating methionine	UNP Q82446
N	428	GLY	-	expression tag	UNP Q82446
N	645	ALA	-	expression tag	UNP Q82446
N	646	ALA	-	expression tag	UNP Q82446
N	647	ALA	-	expression tag	UNP Q82446
N	648	GLU	-	expression tag	UNP Q82446
N	649	LEU	-	expression tag	UNP Q82446

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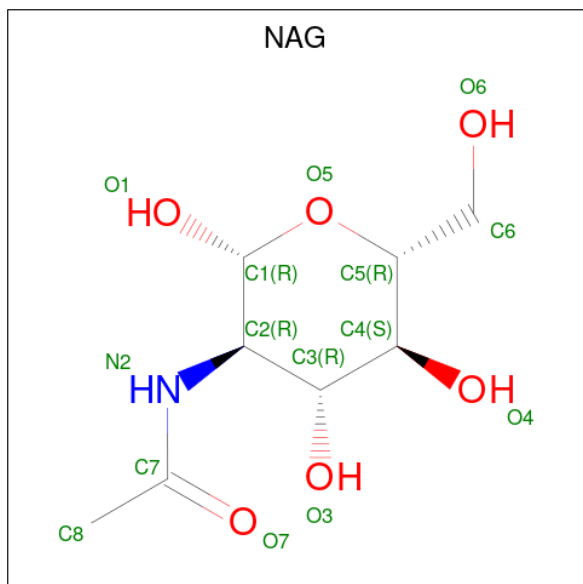
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Chain	Residue	Modelled	Actual	Comment	Reference
N	650	ALA	-	expression tag	UNP Q82446
N	651	LEU	-	expression tag	UNP Q82446
N	652	VAL	-	expression tag	UNP Q82446
N	653	PRO	-	expression tag	UNP Q82446
N	654	ARG	-	expression tag	UNP Q82446
M	427	MET	-	initiating methionine	UNP Q82446
M	428	GLY	-	expression tag	UNP Q82446
M	645	ALA	-	expression tag	UNP Q82446
M	646	ALA	-	expression tag	UNP Q82446
M	647	ALA	-	expression tag	UNP Q82446
M	648	GLU	-	expression tag	UNP Q82446
M	649	LEU	-	expression tag	UNP Q82446
M	650	ALA	-	expression tag	UNP Q82446
M	651	LEU	-	expression tag	UNP Q82446
M	652	VAL	-	expression tag	UNP Q82446
M	653	PRO	-	expression tag	UNP Q82446
M	654	ARG	-	expression tag	UNP Q82446
S	427	MET	-	initiating methionine	UNP Q82446
S	428	GLY	-	expression tag	UNP Q82446
S	645	ALA	-	expression tag	UNP Q82446
S	646	ALA	-	expression tag	UNP Q82446
S	647	ALA	-	expression tag	UNP Q82446
S	648	GLU	-	expression tag	UNP Q82446
S	649	LEU	-	expression tag	UNP Q82446
S	650	ALA	-	expression tag	UNP Q82446
S	651	LEU	-	expression tag	UNP Q82446
S	652	VAL	-	expression tag	UNP Q82446
S	653	PRO	-	expression tag	UNP Q82446
S	654	ARG	-	expression tag	UNP Q82446
T	427	MET	-	initiating methionine	UNP Q82446
T	428	GLY	-	expression tag	UNP Q82446
T	645	ALA	-	expression tag	UNP Q82446
T	646	ALA	-	expression tag	UNP Q82446
T	647	ALA	-	expression tag	UNP Q82446
T	648	GLU	-	expression tag	UNP Q82446
T	649	LEU	-	expression tag	UNP Q82446
T	650	ALA	-	expression tag	UNP Q82446
T	651	LEU	-	expression tag	UNP Q82446
T	652	VAL	-	expression tag	UNP Q82446
T	653	PRO	-	expression tag	UNP Q82446
T	654	ARG	-	expression tag	UNP Q82446

- Molecule 2 is a protein called PL-2 scFv chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1726	1087	290	342	7			
2	E	224	Total	C	N	O	S	0	0	0
			1727	1087	288	345	7			
2	K	223	Total	C	N	O	S	0	0	0
			1726	1087	290	342	7			
2	I	225	Total	C	N	O	S	0	0	0
			1738	1093	292	346	7			
2	Q	93	Total	C	N	O	S	0	0	0
			746	482	122	138	4			
2	O	212	Total	C	N	O	S	0	0	0
			1651	1043	276	325	7			
2	W	105	Total	C	N	O	S	0	0	0
			853	548	141	159	5			
2	U	222	Total	C	N	O	S	0	0	0
			1719	1082	289	341	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		

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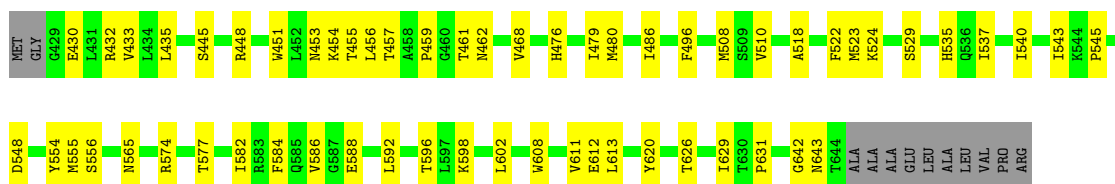
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	I	1	14	8	1	5	0	0

### 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.

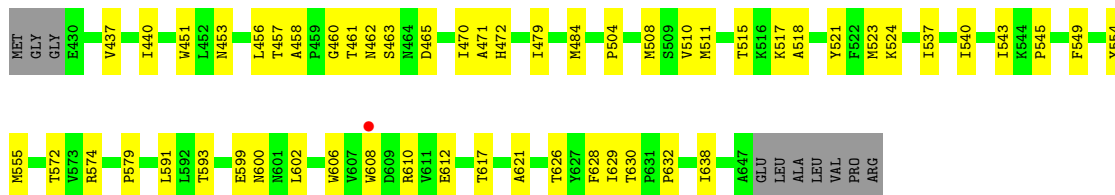
- Molecule 1: Capsid polyprotein VP90

Chain A: 



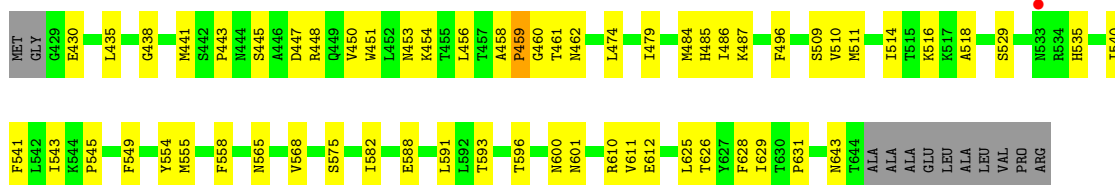
- Molecule 1: Capsid polyprotein VP90

Chain B: 



- Molecule 1: Capsid polyprotein VP90

Chain H: 



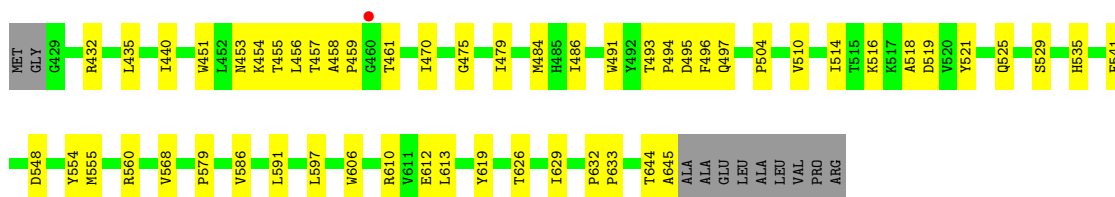
- Molecule 1: Capsid polyprotein VP90

Chain G: 

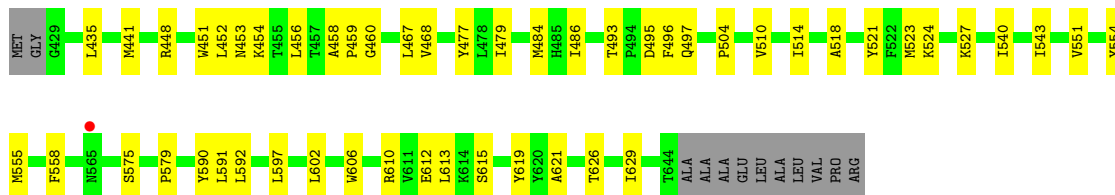




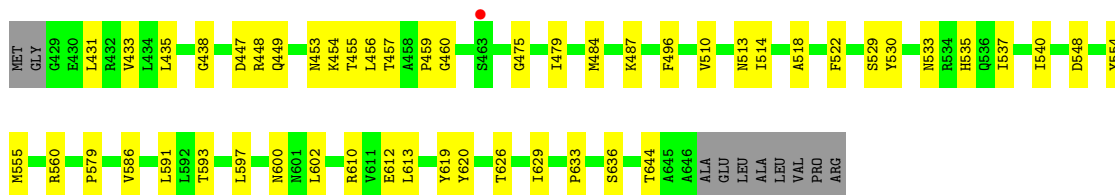
• Molecule 1: Capsid polyprotein VP90



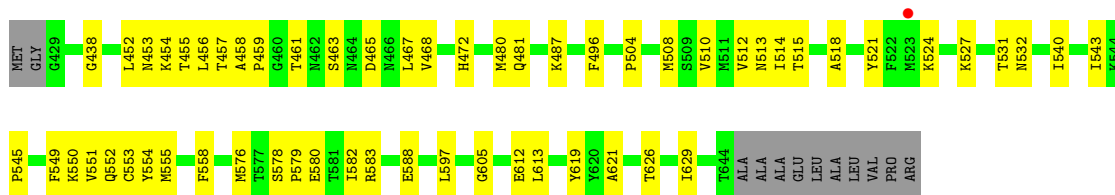
• Molecule 1: Capsid polyprotein VP90



• Molecule 1: Capsid polyprotein VP90



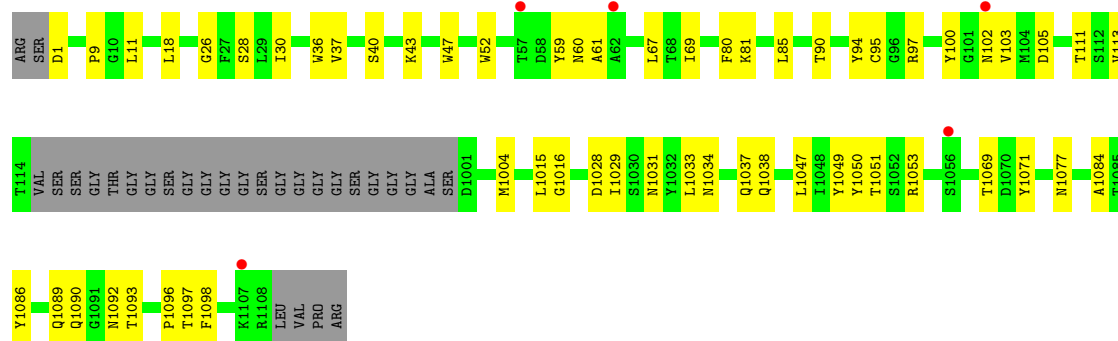
• Molecule 1: Capsid polyprotein VP90



• Molecule 2: PL-2 scFv chain







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.00Å 200.00Å 157.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 50.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	88.1 (50.00-3.25) 81.6 (50.00-3.25)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 3.25Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.241 , 0.288 0.243 , 0.289	Depositor DCC
$R_{free}$ test set	4185 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.5	Xtrriage
Anisotropy	0.523	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 92.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.417 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	25943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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	0.20	0/1792	0.44	0/2441
1	B	0.19	0/1803	0.42	0/2457
1	G	0.20	0/1807	0.48	2/2462 (0.1%)
1	H	0.21	0/1792	0.44	0/2441
1	M	0.16	0/1792	0.43	0/2441
1	N	0.17	0/1797	0.44	0/2448
1	S	0.18	0/1802	0.48	2/2455 (0.1%)
1	T	0.18	0/1792	0.45	0/2441
2	C	0.27	0/1765	0.49	0/2395
2	E	0.18	0/1766	0.45	1/2397 (0.0%)
2	I	0.18	0/1777	0.45	0/2411
2	K	0.22	0/1765	0.45	0/2395
2	O	0.21	0/1686	0.50	1/2283 (0.0%)
2	Q	0.12	0/764	0.39	0/1031
2	U	0.17	0/1758	0.42	0/2385
2	W	0.17	0/874	0.49	1/1179 (0.1%)
All	All	0.19	0/26532	0.45	7/36062 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
2	O	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	100	TYR	N-CA-C	6.53	123.65	113.72
2	W	1093	THR	CB-CA-C	-6.33	107.53	115.89
2	E	100	TYR	N-CA-C	6.13	122.83	113.51
1	S	513	ASN	CA-C-N	-6.13	114.52	123.10
1	S	513	ASN	C-N-CA	-6.13	114.52	123.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	459	PRO	Peptide
2	O	111	THR	Peptide

## 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	1745	0	1709	46	0
1	B	1756	0	1721	38	0
1	G	1760	0	1724	47	0
1	H	1745	0	1709	44	0
1	M	1745	0	1709	39	0
1	N	1750	0	1714	38	0
1	S	1755	0	1719	35	0
1	T	1745	0	1709	55	0
2	C	1726	0	1661	41	0
2	E	1727	0	1658	49	0
2	I	1738	0	1671	36	0
2	K	1726	0	1661	39	0
2	O	1651	0	1587	49	0
2	Q	746	0	701	14	0
2	U	1719	0	1653	47	0
2	W	853	0	788	22	0
3	C	14	0	13	1	0
3	E	14	0	13	0	0
3	I	14	0	13	0	0
3	K	14	0	13	1	0
All	All	25943	0	25146	585	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 11.

The worst 5 of 585 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:H:514:ILE:HD11	2:K:30:ILE:HB	1.54	0.90
1:T:554:TYR:HA	1:T:579:PRO:HA	1.55	0.89
1:S:484:MET:HB3	1:S:591:LEU:HB3	1.56	0.88
1:B:461:THR:HG22	1:B:463:SER:H	1.42	0.84
1:G:461:THR:HG22	1:G:462:ASN:H	1.42	0.83

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	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
1	B	216/228 (95%)	205 (95%)	11 (5%)	0	100	100
1	G	217/228 (95%)	207 (95%)	10 (5%)	0	100	100
1	H	214/228 (94%)	206 (96%)	8 (4%)	0	100	100
1	M	214/228 (94%)	204 (95%)	10 (5%)	0	100	100
1	N	215/228 (94%)	201 (94%)	14 (6%)	0	100	100
1	S	216/228 (95%)	204 (94%)	12 (6%)	0	100	100
1	T	214/228 (94%)	202 (94%)	12 (6%)	0	100	100
2	C	219/251 (87%)	213 (97%)	6 (3%)	0	100	100
2	E	220/251 (88%)	211 (96%)	9 (4%)	0	100	100
2	I	221/251 (88%)	212 (96%)	9 (4%)	0	100	100
2	K	219/251 (87%)	209 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	202/251 (80%)	194 (96%)	8 (4%)	0	100	100
2	Q	81/251 (32%)	69 (85%)	12 (15%)	0	100	100
2	U	218/251 (87%)	209 (96%)	9 (4%)	0	100	100
2	W	91/251 (36%)	84 (92%)	7 (8%)	0	100	100
All	All	3191/3832 (83%)	3036 (95%)	155 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	197/204 (97%)	197 (100%)	0	100	100
1	B	197/204 (97%)	197 (100%)	0	100	100
1	G	197/204 (97%)	197 (100%)	0	100	100
1	H	197/204 (97%)	197 (100%)	0	100	100
1	M	197/204 (97%)	197 (100%)	0	100	100
1	N	197/204 (97%)	197 (100%)	0	100	100
1	S	197/204 (97%)	197 (100%)	0	100	100
1	T	197/204 (97%)	197 (100%)	0	100	100
2	C	193/206 (94%)	193 (100%)	0	100	100
2	E	194/206 (94%)	194 (100%)	0	100	100
2	I	195/206 (95%)	195 (100%)	0	100	100
2	K	193/206 (94%)	193 (100%)	0	100	100
2	O	185/206 (90%)	185 (100%)	0	100	100
2	Q	82/206 (40%)	82 (100%)	0	100	100
2	U	192/206 (93%)	192 (100%)	0	100	100
2	W	93/206 (45%)	93 (100%)	0	100	100
All	All	2903/3280 (88%)	2903 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	1090	GLN
2	U	1080	GLN
1	T	552	GLN
2	U	1034	ASN
1	G	513	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	NAG	E	1201	2	14,14,15	0.34	0	17,19,21	0.59	0
3	NAG	I	1201	2	14,14,15	0.27	0	17,19,21	0.52	0
3	NAG	K	1201	2	14,14,15	0.34	0	17,19,21	0.46	0
3	NAG	C	1201	2	14,14,15	0.40	0	17,19,21	0.47	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
3	NAG	E	1201	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1201	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1201	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1201	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1201	NAG	O5-C5-C6-O6
3	K	1201	NAG	O5-C5-C6-O6
3	I	1201	NAG	C4-C5-C6-O6
3	C	1201	NAG	O5-C5-C6-O6
3	C	1201	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1201	NAG	1	0
3	C	1201	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	216/228 (94%)	-0.57	0 <b>100</b> <b>100</b>	50, 81, 124, 168	0
1	B	218/228 (95%)	-0.19	1 (0%) 87 76	59, 106, 136, 152	0
1	G	219/228 (96%)	-0.13	2 (0%) 81 64	64, 108, 146, 163	0
1	H	216/228 (94%)	-0.50	1 (0%) 87 76	52, 82, 127, 165	0
1	M	216/228 (94%)	-0.32	1 (0%) 87 76	66, 103, 135, 151	0
1	N	217/228 (95%)	-0.61	1 (0%) 87 76	59, 91, 129, 147	0
1	S	218/228 (95%)	-0.61	1 (0%) 87 76	58, 92, 131, 149	0
1	T	216/228 (94%)	-0.26	1 (0%) 87 76	70, 103, 138, 164	0
2	C	223/251 (88%)	-0.62	1 (0%) 88 79	35, 70, 122, 147	3 (1%)
2	E	224/251 (89%)	0.07	4 (1%) 67 48	58, 121, 149, 166	3 (1%)
2	I	225/251 (89%)	0.15	3 (1%) 75 56	75, 126, 157, 175	3 (1%)
2	K	223/251 (88%)	-0.59	0 <b>100</b> <b>100</b>	37, 71, 125, 146	3 (1%)
2	O	212/251 (84%)	0.16	3 (1%) 73 54	66, 131, 155, 167	3 (1%)
2	Q	93/251 (37%)	0.07	1 (1%) 78 61	120, 145, 163, 172	0
2	U	222/251 (88%)	0.24	5 (2%) 61 41	64, 129, 166, 193	3 (1%)
2	W	105/251 (41%)	0.05	1 (0%) 79 63	114, 145, 162, 173	0
All	All	3263/3832 (85%)	-0.25	26 (0%) <b>82</b> <b>67</b>	35, 106, 151, 193	18 (0%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2	VAL	3.9
1	G	474	LEU	2.9
2	I	23	THR	2.8
2	O	23	THR	2.7
2	O	1094	PHE	2.5

## 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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	1201	14/15	0.94	0.12	138,153,158,158	0
3	NAG	I	1201	14/15	0.94	0.10	133,147,156,157	0
3	NAG	C	1201	14/15	0.95	0.14	146,163,170,174	0
3	NAG	K	1201	14/15	0.97	0.09	140,179,188,188	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.