



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2022 – 06:29 PM JST

PDB ID : 7FC5  
Title : Crystal structure of SARS-CoV-2 RBD and horse ACE2  
Authors : Wang, X.Q.; Lan, J.; Ge, J.W.  
Deposited on : 2021-07-13  
Resolution : 2.89 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 : 2.28.1  
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) : 2.28.1

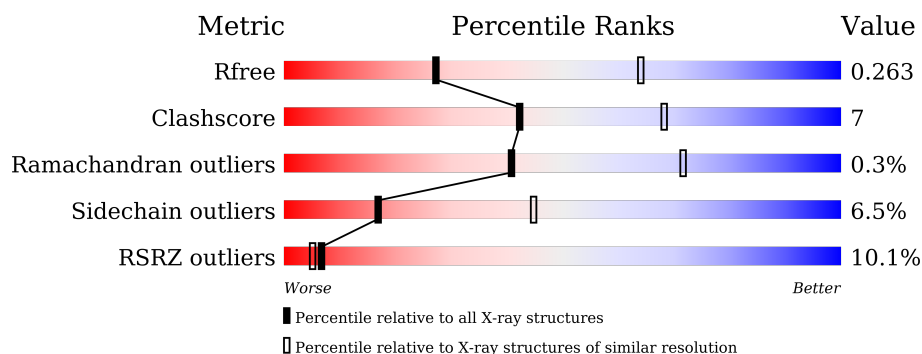
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	E	197	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>25%</div> <div>..</div> </div> </div>
2	A	597	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </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
3	NAG	E	601	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6474 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.

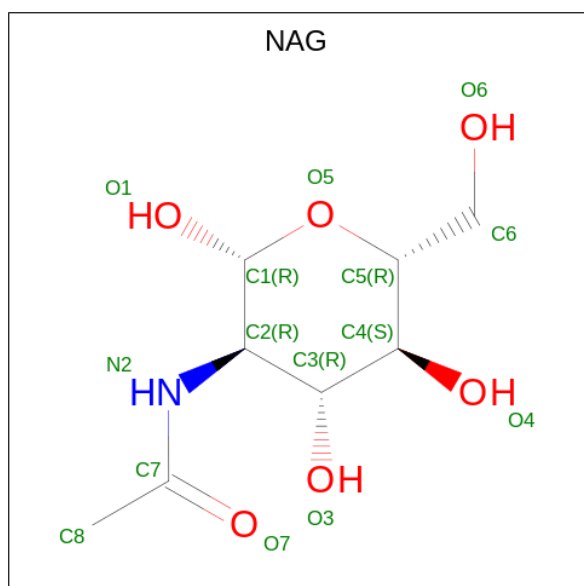
- Molecule 1 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	195	Total	C	N	O	S	0	2	0
			1551	995	258	290	8			

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	596	Total	C	N	O	S	0	0	0
			4853	3100	804	920	29			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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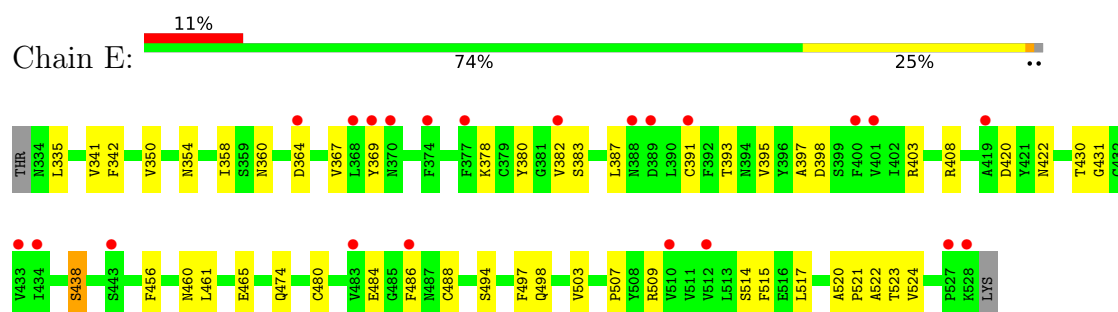
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

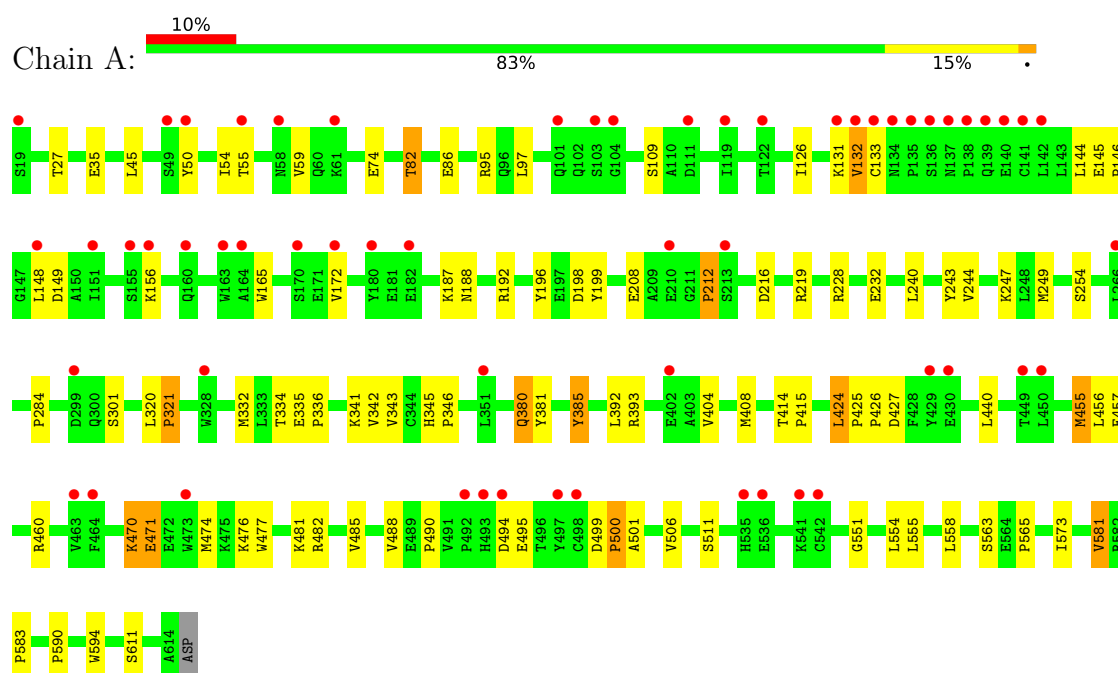
### 3 Residue-property plots

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: Spike protein S1



#### • Molecule 2: Angiotensin-converting enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.17Å 196.17Å 144.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 2.89 49.04 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.4 (46.73-2.89) 95.8 (49.04-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, $R_{free}$	0.229 , 0.259 0.243 , 0.263	Depositor DCC
$R_{free}$ test set	1419 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	1.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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	E	0.57	0/1601	0.73	0/2178
2	A	0.61	0/4989	0.79	2/6775 (0.0%)
All	All	0.60	0/6590	0.78	2/8953 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	95	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	A	321	PRO	CA-N-CD	-5.77	103.43	111.50

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	E	1551	0	1475	30	0
2	A	4853	0	4639	60	0
3	A	56	0	52	0	0
3	E	14	0	13	4	0
All	All	6474	0	6179	87	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 7.

All (87) 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:E:382:VAL:CG1	1:E:387:LEU:HD21	2.13	0.79
1:E:367:VAL:CG1	3:E:601:NAG:O3	2.31	0.78
1:E:382:VAL:HG11	1:E:387:LEU:HD21	1.70	0.74
2:A:332:MET:SD	2:A:342:VAL:HG11	2.31	0.71
2:A:336:PRO:HG3	2:A:342:VAL:CG2	2.21	0.70
2:A:336:PRO:HG3	2:A:342:VAL:HG21	1.73	0.70
2:A:482:ARG:HE	2:A:488:VAL:HG23	1.56	0.70
1:E:367:VAL:HG13	3:E:601:NAG:O3	1.96	0.65
1:E:354:ASN:O	1:E:398:ASP:HA	2.01	0.60
1:E:486:PHE:CE1	2:A:82:THR:HG21	2.37	0.60
2:A:50:TYR:CE1	2:A:59:VAL:HG22	2.38	0.59
1:E:382:VAL:HG13	1:E:387:LEU:HD21	1.84	0.59
1:E:342:PHE:HB2	3:E:601:NAG:H82	1.83	0.59
2:A:55:THR:O	2:A:59:VAL:HG23	2.03	0.59
2:A:320:LEU:HD22	2:A:555:LEU:HG	1.85	0.58
1:E:461:LEU:HD22	1:E:465:GLU:HB3	1.85	0.58
1:E:341:VAL:HG11	1:E:397:ALA:HB1	1.86	0.57
1:E:420:ASP:HB3	1:E:460:ASN:OD1	2.06	0.55
2:A:342:VAL:HG12	2:A:343:VAL:O	2.07	0.55
2:A:336:PRO:CG	2:A:342:VAL:HG21	2.37	0.55
1:E:521:PRO:O	1:E:523:THR:HG23	2.07	0.55
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.88	0.54
1:E:335:LEU:HD11	1:E:364:ASP:HB2	1.92	0.52
2:A:499:ASP:H	2:A:500:PRO:HD2	1.74	0.51
1:E:486:PHE:HE1	2:A:82:THR:HG21	1.75	0.51
2:A:228:ARG:O	2:A:232:GLU:HG3	2.12	0.50
2:A:336:PRO:CD	2:A:342:VAL:HG21	2.42	0.49
1:E:358:ILE:HB	1:E:395:VAL:HB	1.94	0.49
1:E:438:SER:OG	1:E:509:ARG:HG3	2.12	0.49
2:A:144:LEU:HA	2:A:148:LEU:HB2	1.94	0.48
2:A:392:LEU:HD13	2:A:563:SER:HA	1.96	0.48
1:E:391:CYS:HA	1:E:524:VAL:O	2.14	0.47
2:A:501:ALA:HA	2:A:506:VAL:HB	1.95	0.47
2:A:335:GLU:HG3	2:A:336:PRO:HD2	1.96	0.47
1:E:367:VAL:HG11	3:E:601:NAG:O3	2.13	0.47
2:A:385:TYR:O	2:A:393:ARG:HG2	2.16	0.46
2:A:474:MET:HE1	2:A:499:ASP:HB2	1.97	0.46
1:E:456:PHE:CE1	2:A:27:THR:HG23	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:380:GLN:HE21	2:A:380:GLN:HB2	1.36	0.45
2:A:54:ILE:HB	2:A:341:LYS:HB2	1.97	0.45
2:A:187:LYS:HD2	2:A:199:TYR:CZ	2.51	0.45
2:A:284:PRO:HB3	2:A:594:TRP:CH2	2.50	0.45
2:A:424:LEU:HA	2:A:425:PRO:HD2	1.77	0.45
2:A:86:GLU:H	2:A:86:GLU:HG3	1.48	0.45
2:A:404:VAL:O	2:A:408:MET:HG2	2.17	0.45
2:A:455:MET:HE2	2:A:485:VAL:HG21	1.98	0.45
2:A:192:ARG:HA	2:A:196:TYR:O	2.17	0.45
1:E:497:PHE:CD1	1:E:507:PRO:HD3	2.51	0.45
2:A:284:PRO:HB3	2:A:594:TRP:CZ2	2.52	0.45
2:A:240:LEU:O	2:A:244:VAL:HG23	2.17	0.45
1:E:484:GLU:HG3	1:E:488:CYS:O	2.18	0.44
2:A:345:HIS:HA	2:A:346:PRO:HD3	1.72	0.44
1:E:393:THR:HG21	1:E:520:ALA:HB3	1.99	0.44
1:E:431:GLY:HA2	1:E:515:PHE:HD2	1.83	0.44
2:A:342:VAL:HG12	2:A:343:VAL:N	2.33	0.44
2:A:471:GLU:H	2:A:471:GLU:HG2	1.54	0.44
1:E:393:THR:HA	1:E:522:ALA:HA	1.99	0.44
1:E:393:THR:HG21	1:E:520:ALA:CB	2.48	0.43
2:A:455:MET:SD	2:A:481:LYS:HG2	2.58	0.43
2:A:208:GLU:HB2	2:A:219:ARG:HG2	1.98	0.43
2:A:243:TYR:O	2:A:247:LYS:HG2	2.18	0.43
2:A:132:VAL:HG22	2:A:148:LEU:HD21	2.00	0.43
1:E:382:VAL:HG21	1:E:515:PHE:CD2	2.54	0.43
2:A:45:LEU:HD23	2:A:45:LEU:HA	1.83	0.43
1:E:380:TYR:O	1:E:430:THR:HA	2.20	0.42
2:A:474:MET:HE2	2:A:474:MET:HB3	1.74	0.42
2:A:494:ASP:HB2	2:A:495:GLU:H	1.70	0.42
2:A:212:PRO:HD3	2:A:565:PRO:HG2	2.01	0.42
2:A:336:PRO:HG3	2:A:342:VAL:HG23	1.99	0.42
2:A:499:ASP:N	2:A:500:PRO:HD2	2.35	0.41
2:A:320:LEU:CD2	2:A:555:LEU:HG	2.50	0.41
1:E:461:LEU:HD23	1:E:461:LEU:HA	1.92	0.41
2:A:126:ILE:HG22	2:A:172:VAL:HG13	2.02	0.41
2:A:425:PRO:HA	2:A:426:PRO:HD3	1.89	0.41
2:A:165:TRP:CH2	2:A:490:PRO:HD2	2.55	0.41
2:A:414:THR:HA	2:A:415:PRO:HD3	1.88	0.41
2:A:188:ASN:O	2:A:192:ARG:HG3	2.21	0.41
2:A:470:LYS:HB2	2:A:470:LYS:HE3	1.80	0.41
2:A:476:LYS:O	2:A:477:TRP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:551:GLY:O	2:A:555:LEU:HB2	2.21	0.41
2:A:555:LEU:HD23	2:A:555:LEU:HA	1.75	0.40
2:A:131:LYS:HB3	2:A:131:LYS:HE3	1.86	0.40
2:A:554:LEU:O	2:A:558:LEU:HG	2.22	0.40
2:A:145:GLU:HA	2:A:146:PRO:HA	1.84	0.40
2:A:232:GLU:HB2	2:A:581:VAL:HG21	2.04	0.40
1:E:474:GLN:HG3	1:E:480:CYS:SG	2.62	0.40
2:A:460:ARG:NH2	2:A:506:VAL:HA	2.36	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	E	195/197 (99%)	185 (95%)	10 (5%)	0	100	100
2	A	594/597 (100%)	562 (95%)	30 (5%)	2 (0%)	41	71
All	All	789/794 (99%)	747 (95%)	40 (5%)	2 (0%)	41	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	212	PRO
2	A	321	PRO

### 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	E	170/170 (100%)	158 (93%)	12 (7%)	14	40
2	A	524/525 (100%)	491 (94%)	33 (6%)	18	46
All	All	694/695 (100%)	649 (94%)	45 (6%)	17	45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	360	ASN
1	E	369	TYR
1	E	378	LYS
1	E	383	SER
1	E	403	ARG
1	E	408	ARG
1	E	438	SER
1	E	494	SER
1	E	498	GLN
1	E	503	VAL
1	E	514	SER
1	E	517	LEU
2	A	35	GLU
2	A	74	GLU
2	A	82	THR
2	A	97	LEU
2	A	109	SER
2	A	132	VAL
2	A	133	CYS
2	A	149	ASP
2	A	156	LYS
2	A	198	ASP
2	A	216	ASP
2	A	249	MET
2	A	254	SER
2	A	301	SER
2	A	334	THR
2	A	380	GLN
2	A	381	TYR
2	A	385	TYR
2	A	424	LEU
2	A	427	ASP
2	A	440	LEU
2	A	455	MET

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Mol	Chain	Res	Type
2	A	456	LEU
2	A	457	GLU
2	A	470	LYS
2	A	471	GLU
2	A	500	PRO
2	A	511	SER
2	A	573	ILE
2	A	581	VAL
2	A	583	PRO
2	A	590	PRO
2	A	611	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	380	GLN
2	A	552	GLN

### 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](#)

5 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	601	1	14,14,15	0.39	0	17,19,21	0.81	0
3	NAG	A	701	2	14,14,15	0.33	0	17,19,21	1.31	3 (17%)
3	NAG	A	703	2	14,14,15	0.41	0	17,19,21	0.94	0
3	NAG	A	704	2	14,14,15	0.48	0	17,19,21	1.58	2 (11%)
3	NAG	A	702	2	14,14,15	0.73	0	17,19,21	1.27	1 (5%)

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	601	1	-	2/6/23/26	0/1/1/1
3	NAG	A	701	2	-	4/6/23/26	0/1/1/1
3	NAG	A	703	2	-	2/6/23/26	0/1/1/1
3	NAG	A	704	2	-	2/6/23/26	0/1/1/1
3	NAG	A	702	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	NAG	O5-C5-C6	4.08	113.60	107.20
3	A	701	NAG	C2-N2-C7	3.21	127.48	122.90
3	A	702	NAG	C4-C3-C2	-3.18	106.36	111.02
3	A	704	NAG	C1-C2-N2	-2.93	105.48	110.49
3	A	701	NAG	C1-O5-C5	2.04	114.95	112.19
3	A	701	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	NAG	C8-C7-N2-C2
3	A	704	NAG	O7-C7-N2-C2
3	A	701	NAG	C8-C7-N2-C2
3	A	701	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	703	NAG	C8-C7-N2-C2
3	A	703	NAG	O7-C7-N2-C2
3	E	601	NAG	O5-C5-C6-O6
3	A	701	NAG	C1-C2-N2-C7
3	E	601	NAG	C4-C5-C6-O6
3	A	701	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	NAG	4	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	E	195/197 (98%)	0.66	22 (11%) <b>5</b> <b>4</b>	30, 52, 96, 110	0
2	A	596/597 (99%)	0.64	58 (9%) <b>7</b> <b>6</b>	28, 47, 78, 135	0
All	All	791/794 (99%)	0.64	80 (10%) <b>7</b> <b>5</b>	28, 49, 85, 135	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	136	SER	7.6
2	A	163	TRP	6.5
2	A	139	GLN	6.4
2	A	140	GLU	5.4
2	A	172	VAL	4.6
2	A	103	SER	4.5
2	A	536	GLU	4.4
2	A	498	CYS	4.4
2	A	138	PRO	4.3
2	A	156	LYS	4.0
2	A	133	CYS	4.0
2	A	541	LYS	3.9
2	A	492	PRO	3.9
2	A	137	ASN	3.9
2	A	164	ALA	3.8
2	A	141	CYS	3.7
2	A	135	PRO	3.7
1	E	368	LEU	3.6
2	A	210	GLU	3.6
1	E	527	PRO	3.6
2	A	464	PHE	3.5
2	A	148	LEU	3.5
2	A	134	ASN	3.4
2	A	132	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	A	429	TYR	3.4
2	A	497	TYR	3.2
1	E	382	VAL	3.2
2	A	180	TYR	3.2
2	A	493	HIS	3.2
2	A	104	GLY	3.1
1	E	388	ASN	3.0
1	E	433	VAL	3.0
2	A	494	ASP	2.9
2	A	170	SER	2.9
2	A	101	GLN	2.8
1	E	377	PHE	2.8
2	A	182	GLU	2.7
1	E	401	VAL	2.7
2	A	142	LEU	2.7
1	E	400	PHE	2.7
1	E	483	VAL	2.7
2	A	49	SER	2.6
1	E	512	VAL	2.6
1	E	486	PHE	2.6
2	A	402	GLU	2.6
1	E	419	ALA	2.6
2	A	58	ASN	2.6
2	A	463	VAL	2.5
2	A	122	THR	2.5
2	A	266	LEU	2.5
2	A	450	LEU	2.5
2	A	473	TRP	2.5
2	A	61	LYS	2.5
1	E	510	VAL	2.5
2	A	131	LYS	2.5
2	A	299	ASP	2.4
2	A	328	TRP	2.4
1	E	369	TYR	2.3
2	A	111	ASP	2.3
2	A	119	ILE	2.3
2	A	50	TYR	2.3
2	A	55	THR	2.2
1	E	364	ASP	2.2
2	A	535	HIS	2.2
1	E	391	CYS	2.2
1	E	370	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	443[A]	SER	2.2
2	A	151	ILE	2.2
2	A	430	GLU	2.1
1	E	389	ASP	2.1
2	A	160	GLN	2.1
2	A	155	SER	2.1
2	A	213	SER	2.1
2	A	449	THR	2.1
1	E	374	PHE	2.1
1	E	434	ILE	2.0
2	A	542	CYS	2.0
2	A	19	SER	2.0
1	E	528	LYS	2.0
2	A	351	LEU	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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	704	14/15	0.65	0.28	30,30,30,30	0
3	NAG	E	601	14/15	0.72	0.41	30,30,30,30	0
3	NAG	A	701	14/15	0.75	0.35	60,79,86,90	0
3	NAG	A	702	14/15	0.82	0.21	65,82,107,109	0
3	NAG	A	703	14/15	0.84	0.16	61,71,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.