



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:05 PM UTC

PDB ID : 7FC5 / pdb_00007fc5
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

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>.

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)
Xtrriage (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

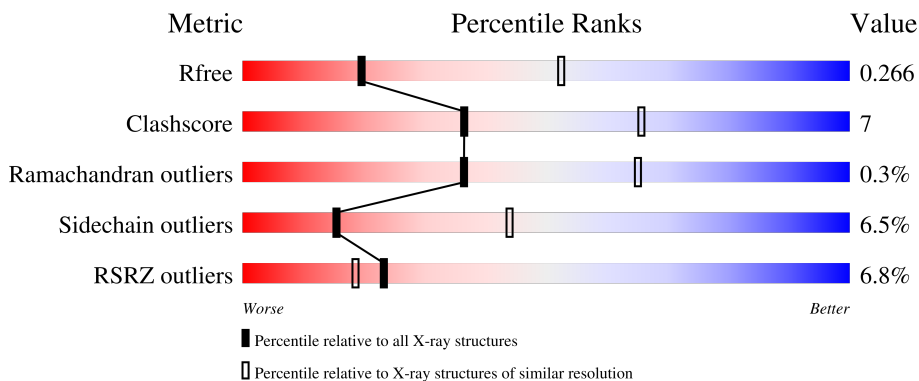
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 ≥ 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	
2	A	597	

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.

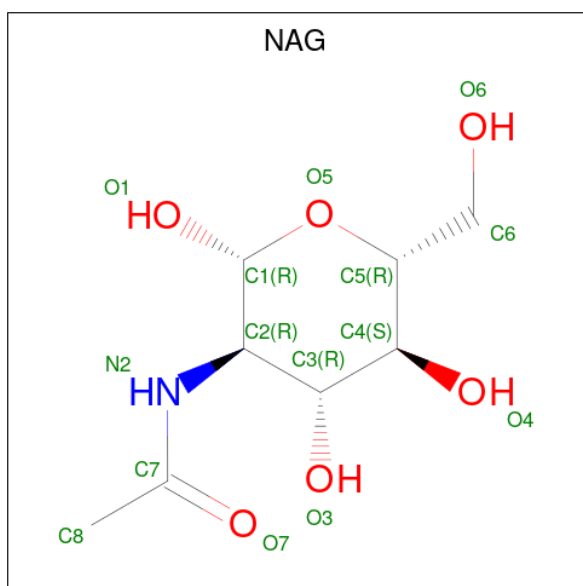
- Molecule 1 is a protein called Spike protein S1.

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

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

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

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



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

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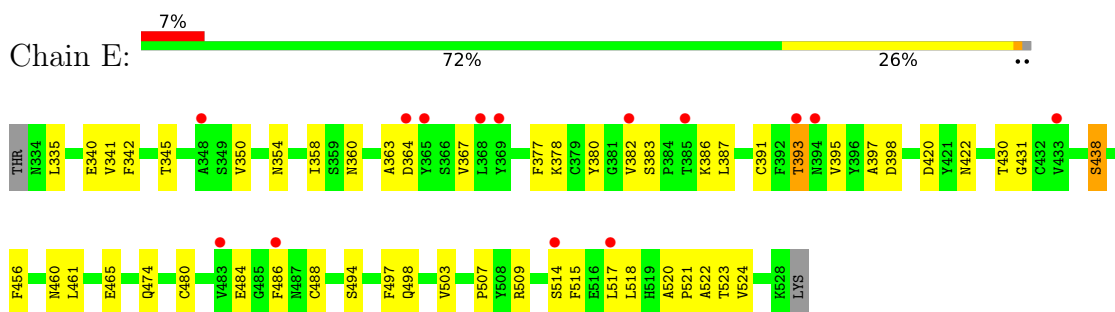
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

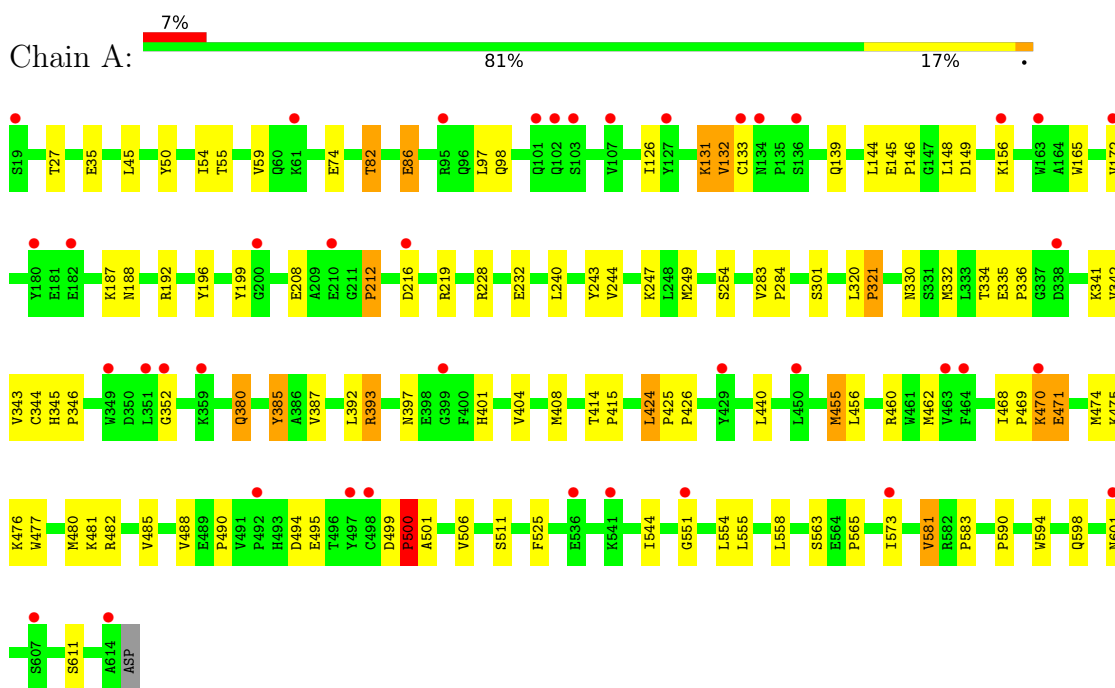
3 Residue-property plots [i](#)

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: 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, α , β , γ	196.17Å 196.17Å 144.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 2.89 46.73 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.4 (46.73-2.89) 95.7 (46.73-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.229 , 0.259 0.243 , 0.266	Depositor DCC
R_{free} test set	1419 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	1.099	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6474	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.59	0/1601	0.92	4/2178 (0.2%)
2	A	0.80	0/4989	1.17	15/6775 (0.2%)
All	All	0.76	0/6590	1.11	19/8953 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	544	ILE	N-CA-C	-8.23	104.68	112.83
2	A	469	PRO	CB-CA-C	-7.06	102.19	111.23
1	E	340	GLU	N-CA-C	-6.98	104.58	113.23
2	A	139	GLN	N-CA-C	-6.58	106.20	114.56
2	A	397	ASN	CA-CB-CG	6.31	118.91	112.60
2	A	321	PRO	CA-N-CD	-6.12	103.43	112.00
2	A	525	PHE	CA-CB-CG	5.90	119.70	113.80
2	A	387	VAL	N-CA-C	-5.87	105.65	112.98
2	A	393	ARG	CB-CA-C	-5.85	102.77	111.72
1	E	393	THR	CB-CA-C	-5.80	101.73	110.90
2	A	330	ASN	CB-CA-C	5.55	118.39	109.07
2	A	344	CYS	N-CA-C	-5.45	106.54	114.12
2	A	601	ASN	N-CA-C	-5.42	105.97	112.59
1	E	363	ALA	N-CA-C	5.31	117.89	109.24
2	A	500	PRO	N-CA-CB	-5.29	97.69	103.25
2	A	598	GLN	N-CA-C	-5.17	106.75	113.16
1	E	377	PHE	CB-CA-C	-5.15	103.88	111.70
2	A	352	GLY	CA-C-O	-5.14	118.69	122.23
2	A	475	LYS	N-CA-C	-5.02	104.81	112.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	64	0
3	A	56	0	52	0	0
3	E	14	0	13	4	0
All	All	6474	0	6179	91	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 (91) 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
2:A:462:MET:HE3	2:A:468:ILE:HD11	1.85	0.57
1:E:341:VAL:HG11	1:E:397:ALA:HB1	1.86	0.57
2:A:474:MET:HE1	2:A:499:ASP:HB2	1.86	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:VAL:HG22	1:E:422:ASN:HB3	1.88	0.54
2:A:455:MET:HG2	2:A:480:MET:HE2	1.89	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:455:MET:HE2	2:A:485:VAL:HG21	1.97	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:476:LYS:O	2:A:477:TRP:C	2.59	0.45
1:E:456:PHE:CE1	2:A:27:THR:HG23	2.52	0.45
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: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:474:MET:HB3	2:A:474:MET:HE3	1.43	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:471:GLU:H	2:A:471:GLU:HG2	1.54	0.44
2:A:342:VAL:HG12	2:A:343:VAL:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:455:MET:HE3	2:A:455:MET:HB3	1.68	0.42
2:A:499:ASP:O	2:A:500:PRO:C	2.63	0.41
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: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%)	36	65
All	All	789/794 (99%)	747 (95%)	40 (5%)	2 (0%)	36	65

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%)	13	40
2	A	524/525 (100%)	491 (94%)	33 (6%)	16	45
All	All	694/695 (100%)	649 (94%)	45 (6%)	15	44

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

Mol	Chain	Res	Type
1	E	345	THR
1	E	360	ASN
1	E	378	LYS
1	E	383	SER
1	E	386	LYS
1	E	438	SER
1	E	494	SER
1	E	498	GLN
1	E	503	VAL
1	E	514	SER
1	E	517	LEU
1	E	518	LEU
2	A	35	GLU
2	A	74	GLU

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Mol	Chain	Res	Type
2	A	82	THR
2	A	86	GLU
2	A	97	LEU
2	A	98	GLN
2	A	131	LYS
2	A	132	VAL
2	A	133	CYS
2	A	149	ASP
2	A	156	LYS
2	A	216	ASP
2	A	249	MET
2	A	254	SER
2	A	283	VAL
2	A	301	SER
2	A	334	THR
2	A	380	GLN
2	A	385	TYR
2	A	401	HIS
2	A	424	LEU
2	A	440	LEU
2	A	455	MET
2	A	456	LEU
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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	360	ASN
1	E	450	ASN
2	A	96	GLN
2	A	102	GLN
2	A	137	ASN
2	A	380	GLN
2	A	524	GLN

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Mol	Chain	Res	Type
2	A	540	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](#)

There are no oligosaccharides 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	A	704	2	14,14,15	0.48	0	17,19,21	1.47	2 (11%)
3	NAG	A	703	2	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
3	NAG	A	701	2	14,14,15	0.32	0	17,19,21	1.36	3 (17%)
3	NAG	A	702	2	14,14,15	0.72	0	17,19,21	1.27	1 (5%)
3	NAG	E	601	1	14,14,15	0.39	0	17,19,21	0.75	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	A	704	2	-	2/6/23/26	0/1/1/1
3	NAG	A	703	2	-	2/6/23/26	0/1/1/1
3	NAG	A	701	2	-	4/6/23/26	0/1/1/1
3	NAG	A	702	2	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	C2-N2-C7	3.42	127.48	122.90
3	A	702	NAG	C4-C3-C2	-3.18	106.36	111.02
3	A	704	NAG	C1-C2-N2	-3.14	105.48	110.43
3	A	704	NAG	O5-C5-C6	3.05	113.60	107.66
3	A	701	NAG	C1-C2-N2	2.21	113.92	110.43
3	A	701	NAG	C1-O5-C5	2.07	114.95	112.19
3	A	703	NAG	C2-N2-C7	-2.03	120.18	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	C1-C2-N2-C7
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
3	A	703	NAG	C8-C7-N2-C2
3	E	601	NAG	O5-C5-C6-O6
3	A	703	NAG	O7-C7-N2-C2
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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	195/197 (98%)	0.68	14 (7%) 21 17	30, 52, 96, 110	2 (1%)
2	A	596/597 (99%)	0.59	40 (6%) 24 19	28, 47, 78, 135	0
All	All	791/794 (99%)	0.61	54 (6%) 23 18	28, 49, 85, 135	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	136	SER	6.1
2	A	614	ALA	5.0
2	A	536	GLU	4.8
2	A	210	GLU	4.5
1	E	517	LEU	4.4
2	A	464	PHE	3.8
1	E	369	TYR	3.5
1	E	393	THR	3.3
2	A	163	TRP	3.2
2	A	541	LYS	3.2
2	A	351	LEU	3.1
2	A	180	TYR	3.1
2	A	429	TYR	3.0
2	A	156	LYS	3.0
2	A	359	LYS	3.0
2	A	349	TRP	2.9
2	A	103	SER	2.9
1	E	394	ASN	2.8
2	A	216	ASP	2.7
2	A	492	PRO	2.6
1	E	514	SER	2.6
2	A	399	GLY	2.6
2	A	107	VAL	2.5
1	E	382	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	463	VAL	2.5
2	A	133	CYS	2.5
2	A	573	ILE	2.5
2	A	182	GLU	2.4
1	E	364	ASP	2.4
2	A	498	CYS	2.4
2	A	352	GLY	2.4
2	A	551	GLY	2.3
2	A	134	ASN	2.3
2	A	450	LEU	2.2
1	E	483	VAL	2.2
1	E	365	TYR	2.2
2	A	19	SER	2.2
1	E	433	VAL	2.2
1	E	368	LEU	2.2
2	A	95	ARG	2.1
2	A	200	GLY	2.1
2	A	601	ASN	2.1
2	A	338	ASP	2.1
2	A	607	SER	2.1
2	A	101	GLN	2.1
2	A	172	VAL	2.1
2	A	470	LYS	2.1
2	A	61	LYS	2.1
1	E	486	PHE	2.1
1	E	348	ALA	2.1
2	A	127	TYR	2.1
2	A	102	GLN	2.0
1	E	385	THR	2.0
2	A	497	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	701	14/15	0.61	0.14	60,79,86,90	0
3	NAG	A	704	14/15	0.64	0.18	30,30,30,30	0
3	NAG	E	601	14/15	0.77	0.21	30,30,30,30	0
3	NAG	A	702	14/15	0.78	0.13	65,82,107,109	0
3	NAG	A	703	14/15	0.84	0.10	61,71,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.