



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 11, 2018 – 12:45 AM EDT

PDB ID : 3KBH
Title : Crystal structure of NL63 respiratory coronavirus receptor-binding domain complexed with its human receptor
Authors : Wu, K.; Li, W.; Peng, G.; Li, F.
Deposited on : 2009-10-20
Resolution : 3.31 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031021
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031021

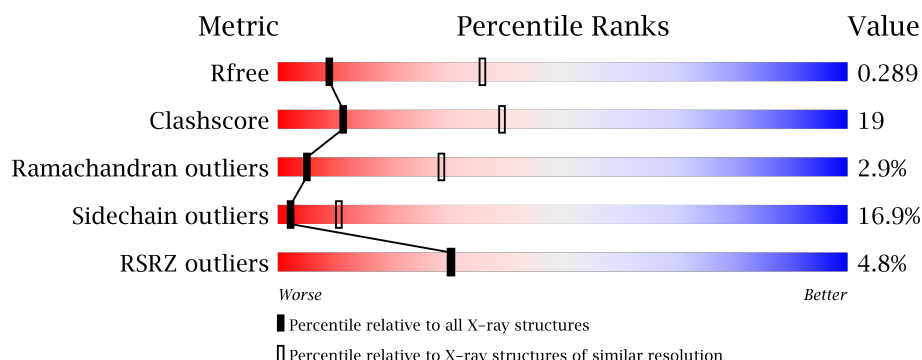
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	111664	1128 (3.38-3.26)
Clashscore	122126	1187 (3.38-3.26)
Ramachandran outliers	120053	1167 (3.38-3.26)
Sidechain outliers	120020	1166 (3.38-3.26)
RSRZ outliers	108989	1094 (3.38-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	597	<div> <div>4%</div> <div>56%</div> <div>36%</div> <div>8%</div> <div>.</div> </div>
1	B	597	<div> <div>5%</div> <div>59%</div> <div>32%</div> <div>8%</div> <div>.</div> </div>
1	C	597	<div> <div>5%</div> <div>57%</div> <div>35%</div> <div>7%</div> <div>.</div> </div>
1	D	597	<div> <div>4%</div> <div>56%</div> <div>35%</div> <div>8%</div> <div>..</div> </div>
2	E	136	<div> <div>%</div> <div>43%</div> <div>24%</div> <div>11%</div> <div>.</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	136	
2	G	136	
2	H	136	

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	A	801	X	-	-	-
3	NAG	B	801	X	-	-	-
3	NAG	C	801	X	-	-	X
3	NAG	D	801	X	-	-	-
3	NAG	E	1486	X	-	-	-
3	NAG	E	1512	X	-	-	-
3	NAG	F	1486	X	-	-	-
3	NAG	F	1512	X	-	-	-
3	NAG	G	1486	X	-	-	-
3	NAG	G	1512	X	-	-	-
3	NAG	H	1486	X	-	-	-
3	NAG	H	1512	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23024 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	B	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	C	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			
1	D	593	Total	C	N	O	S	0	0	0
			4840	3095	802	914	29			

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	F	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	G	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			
2	H	110	Total	C	N	O	S	0	0	0
			860	551	142	161	6			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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	E	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	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

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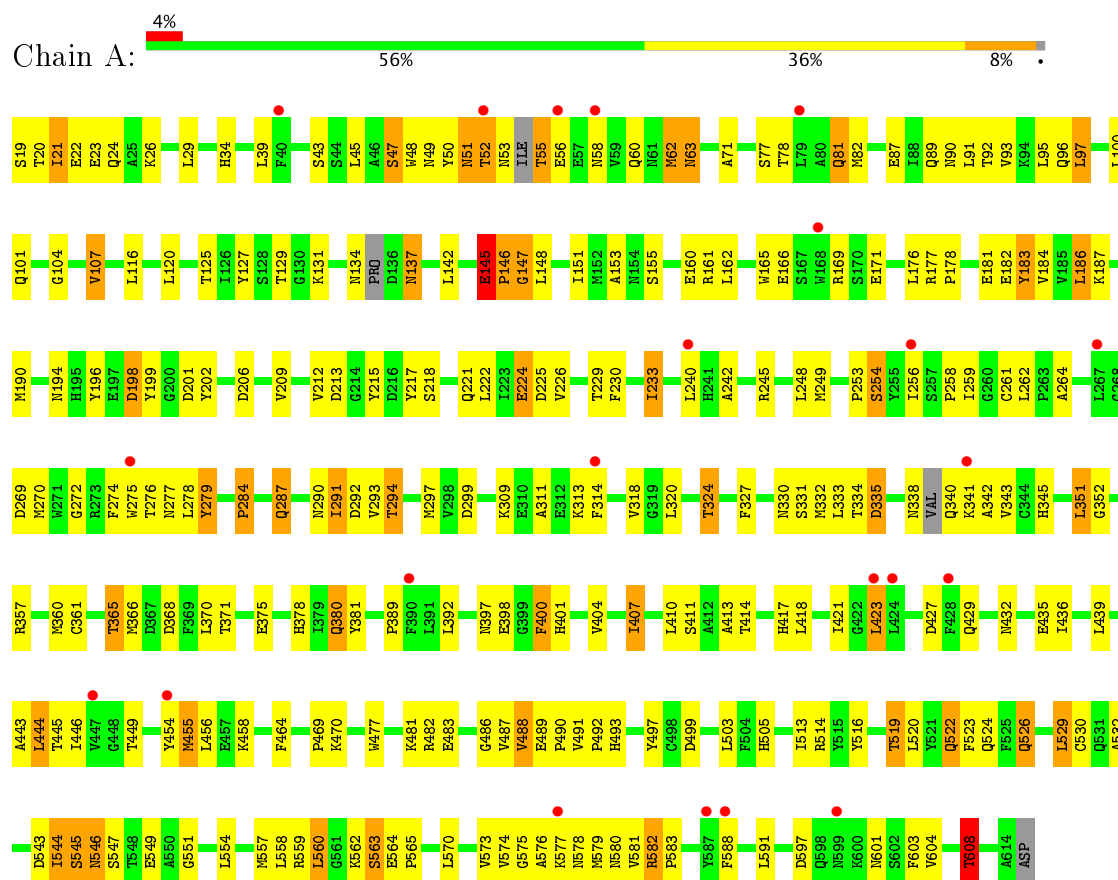
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

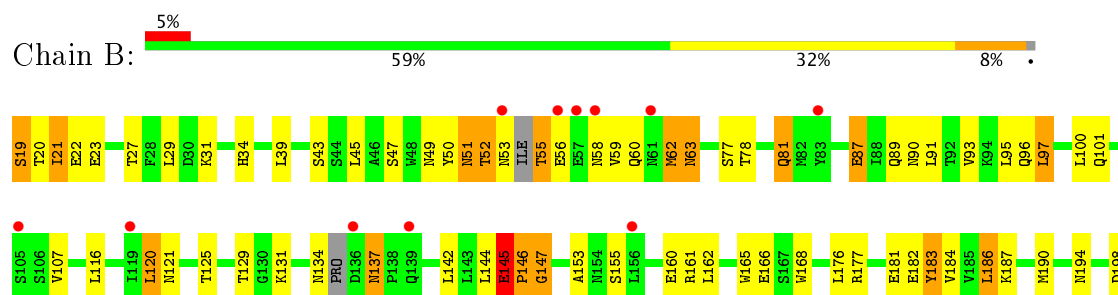
3 Residue-property plots [i](#)

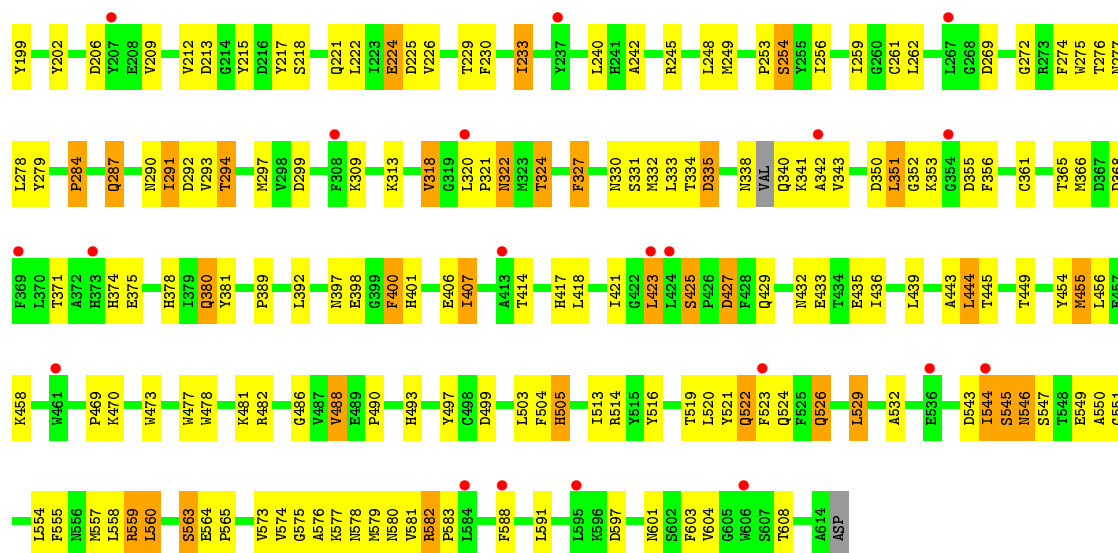
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Angiotensin-converting enzyme 2

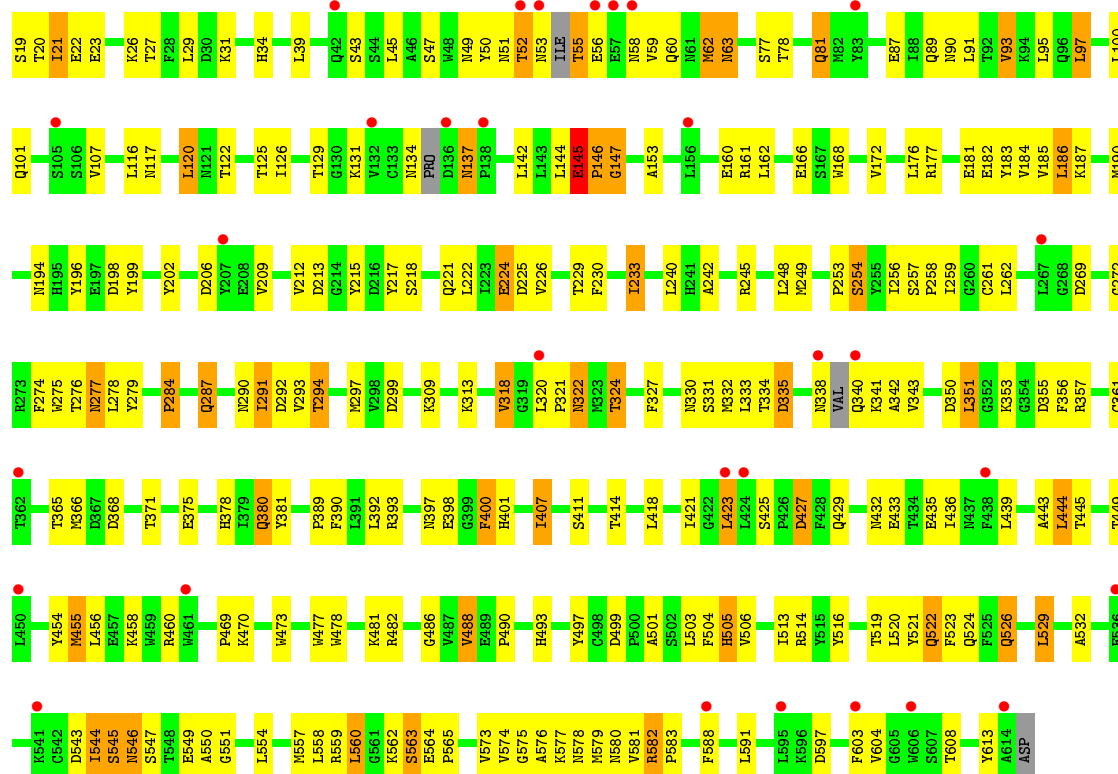


• Molecule 1: Angiotensin-converting enzyme 2

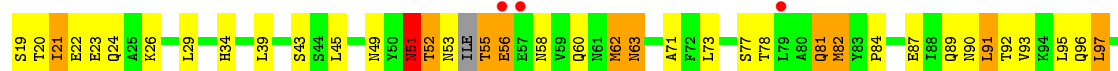


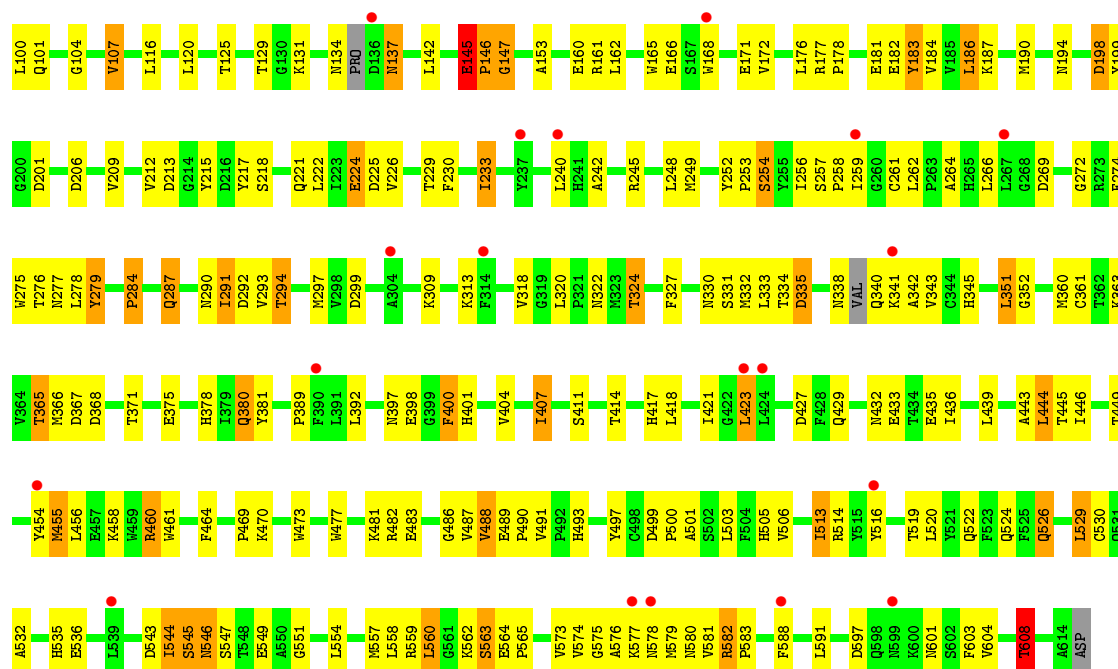


• Molecule 1: Angiotensin-converting enzyme 2

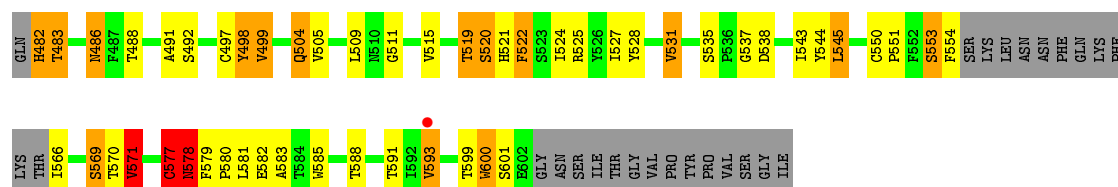
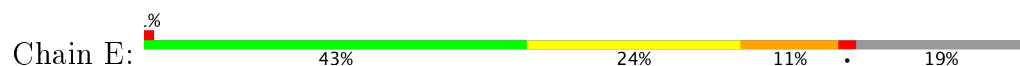


• Molecule 1: Angiotensin-converting enzyme 2

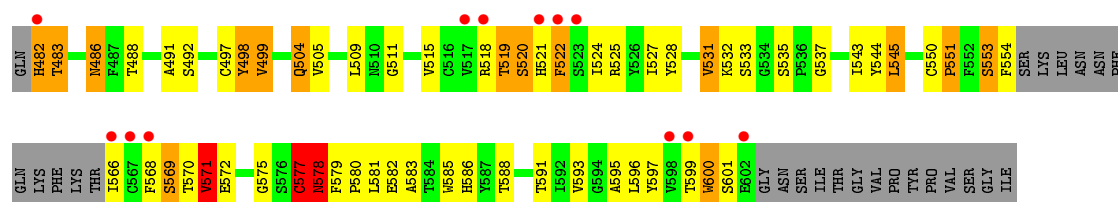




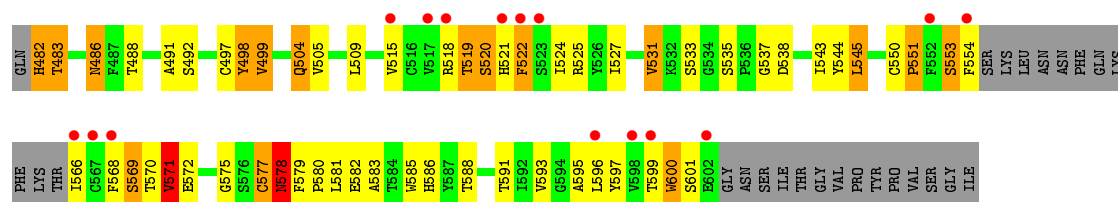
• Molecule 2: Spike glycoprotein



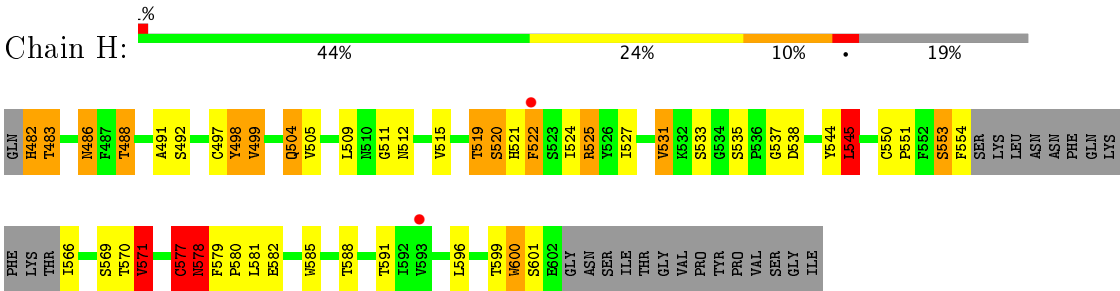
• Molecule 2: Spike glycoprotein



• Molecule 2: Spike glycoprotein



● Molecule 2: Spike glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	77.76 Å 77.76 Å 631.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 3.31 49.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.01-3.31) 88.4 (49.00-3.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.268 , 0.300 0.262 , 0.289	Depositor DCC
R_{free} test set	3040 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.67	0/4973	0.73	0/6750
1	B	0.65	1/4973 (0.0%)	0.71	0/6750
1	C	0.64	1/4973 (0.0%)	0.71	0/6750
1	D	0.66	1/4973 (0.0%)	0.73	1/6750 (0.0%)
2	E	0.86	0/888	0.92	1/1212 (0.1%)
2	F	0.78	0/888	0.90	1/1212 (0.1%)
2	G	0.75	0/888	0.88	0/1212
2	H	0.85	0/888	0.92	2/1212 (0.2%)
All	All	0.68	3/23444 (0.0%)	0.75	5/31848 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	1
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	VAL	CA-CB	6.04	1.67	1.54
1	C	59	VAL	CA-CB	5.67	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	ASN	CB-CG	5.67	1.64	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	577	CYS	CA-CB-SG	5.90	124.61	114.00
2	H	577	CYS	CA-CB-SG	5.54	123.97	114.00
1	D	460	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	F	577	CYS	CA-CB-SG	5.13	123.24	114.00
2	H	545	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLU	Peptide
1	B	145	GLU	Peptide
2	E	520	SER	Peptide
2	E	569	SER	Peptide
2	F	520	SER	Peptide

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	A	4840	0	4607	173	2
1	B	4840	0	4607	162	0
1	C	4840	0	4607	162	0
1	D	4840	0	4607	174	2
2	E	860	0	797	47	0
2	F	860	0	797	50	2
2	G	860	0	797	44	2
2	H	860	0	797	43	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	26	1	0
3	F	28	0	26	1	0
3	G	28	0	26	0	0
3	H	28	0	26	1	0
All	All	23024	0	21824	847	4

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 19.

The worst 5 of 847 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)
2:G:483:THR:HG22	2:G:519:THR:HG23	1.30	1.14
2:E:483:THR:HG22	2:E:519:THR:HG23	1.27	1.13
1:D:51:ASN:HD22	1:D:343:VAL:HG22	1.13	1.10
1:B:145:GLU:HA	1:B:145:GLU:OE1	1.51	1.08
2:F:483:THR:HG22	2:F:519:THR:HG23	1.35	1.07

All (4) 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)
1:A:71:ALA:O	2:G:518:ARG:NH2[3_554]	1.69	0.51
2:F:518:ARG:NH2	1:D:71:ALA:O[3_454]	2.04	0.16
2:F:572:GLU:OE2	1:D:24:GLN:OE1[3_454]	2.09	0.11
1:A:24:GLN:OE1	2:G:572:GLU:OE2[3_554]	2.13	0.07

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	585/597 (98%)	516 (88%)	55 (9%)	14 (2%)	6	32
1	B	585/597 (98%)	515 (88%)	57 (10%)	13 (2%)	7	35
1	C	585/597 (98%)	514 (88%)	57 (10%)	14 (2%)	6	32
1	D	585/597 (98%)	515 (88%)	56 (10%)	14 (2%)	6	32
2	E	106/136 (78%)	87 (82%)	13 (12%)	6 (6%)	2	13
2	F	106/136 (78%)	86 (81%)	13 (12%)	7 (7%)	1	10
2	G	106/136 (78%)	85 (80%)	14 (13%)	7 (7%)	1	10
2	H	106/136 (78%)	86 (81%)	14 (13%)	6 (6%)	2	13
All	All	2764/2932 (94%)	2404 (87%)	279 (10%)	81 (3%)	5	29

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
2	E	499	VAL
2	E	521	HIS
2	E	571	VAL
2	E	578	ASN

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	523/527 (99%)	442 (84%)	81 (16%)	3	14
1	B	523/527 (99%)	442 (84%)	81 (16%)	3	14
1	C	523/527 (99%)	444 (85%)	79 (15%)	3	15
1	D	523/527 (99%)	441 (84%)	82 (16%)	3	14
2	E	98/121 (81%)	74 (76%)	24 (24%)	1	2
2	F	98/121 (81%)	75 (76%)	23 (24%)	1	3
2	G	98/121 (81%)	74 (76%)	24 (24%)	1	2
2	H	98/121 (81%)	71 (72%)	27 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2484/2592 (96%)	2063 (83%)	421 (17%)	2 11

5 of 421 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	498	TYR
1	C	160	GLU
1	D	577	LYS
2	F	522	PHE
1	C	31	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	586	ASN
1	C	81	GLN
1	D	535	HIS
2	F	482	HIS
1	C	24	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	800	1	14,14,15	0.39	0	17,19,21	1.80	3 (17%)
3	NAG	A	801	1	14,14,15	1.06	1 (7%)	17,19,21	2.45	7 (41%)
3	NAG	B	800	1	14,14,15	0.52	0	17,19,21	2.02	6 (35%)
3	NAG	B	801	1	14,14,15	1.15	1 (7%)	17,19,21	2.45	8 (47%)
3	NAG	C	800	1	14,14,15	0.45	0	17,19,21	1.96	6 (35%)
3	NAG	C	801	1	14,14,15	1.10	1 (7%)	17,19,21	2.41	7 (41%)
3	NAG	D	800	1	14,14,15	0.42	0	17,19,21	1.83	3 (17%)
3	NAG	D	801	1	14,14,15	1.03	1 (7%)	17,19,21	2.41	6 (35%)
3	NAG	E	1486	2	14,14,15	0.66	0	17,19,21	0.93	1 (5%)
3	NAG	E	1512	2	14,14,15	0.56	0	17,19,21	2.34	6 (35%)
3	NAG	F	1486	2	14,14,15	0.65	0	17,19,21	0.82	0
3	NAG	F	1512	2	14,14,15	0.68	0	17,19,21	2.38	6 (35%)
3	NAG	G	1486	2	14,14,15	0.65	0	17,19,21	0.79	0
3	NAG	G	1512	2	14,14,15	0.68	0	17,19,21	2.40	6 (35%)
3	NAG	H	1486	2	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
3	NAG	H	1512	2	14,14,15	0.67	0	17,19,21	2.35	6 (35%)

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	800	1	-	0/6/23/26	0/1/1/1
3	NAG	A	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	800	1	-	0/6/23/26	0/1/1/1
3	NAG	B	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	800	1	-	0/6/23/26	0/1/1/1
3	NAG	C	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	800	1	-	0/6/23/26	0/1/1/1
3	NAG	D	801	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	1512	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	1512	2	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	G	1512	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	H	1486	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	H	1512	2	1/1/5/7	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	NAG	C1-C2	3.19	1.56	1.52
3	A	801	NAG	C1-C2	3.24	1.56	1.52
3	C	801	NAG	C1-C2	3.40	1.57	1.52
3	B	801	NAG	C1-C2	3.50	1.57	1.52

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801	NAG	O5-C1-C2	-3.92	106.11	111.52
3	B	801	NAG	O5-C1-C2	-3.56	106.60	111.52
3	D	801	NAG	O5-C1-C2	-3.43	106.79	111.52
3	A	801	NAG	O5-C1-C2	-3.36	106.88	111.52
3	A	801	NAG	C3-C4-C5	-2.88	105.09	110.24

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	1512	NAG	C1
3	E	1512	NAG	C1
3	A	801	NAG	C1
3	F	1486	NAG	C1
3	C	801	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1512	NAG	1	0
3	F	1512	NAG	1	0
3	H	1512	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, 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	A	593/597 (99%)	0.25	22 (3%) 41 39	43, 46, 48, 52	0
1	B	593/597 (99%)	0.37	31 (5%) 27 26	43, 46, 48, 51	0
1	C	593/597 (99%)	0.36	30 (5%) 28 27	43, 46, 48, 52	0
1	D	593/597 (99%)	0.30	22 (3%) 41 39	43, 46, 48, 52	0
2	E	110/136 (80%)	0.26	1 (0%) 84 84	27, 46, 48, 54	0
2	F	110/136 (80%)	0.70	12 (10%) 5 5	27, 46, 48, 54	0
2	G	110/136 (80%)	0.66	15 (13%) 3 3	27, 46, 48, 54	0
2	H	110/136 (80%)	0.28	2 (1%) 68 68	27, 46, 48, 54	0
All	All	2812/2932 (95%)	0.34	135 (4%) 30 30	27, 46, 48, 54	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	523	SER	6.3
1	B	136	ASP	6.3
1	C	136	ASP	6.2
2	F	568	PHE	6.0
2	G	568	PHE	5.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	C	801	14/15	0.50	0.42	65,70,74,75	0
3	NAG	B	801	14/15	0.59	0.37	65,70,74,75	0
3	NAG	F	1512	14/15	0.60	0.32	94,105,108,109	0
3	NAG	H	1512	14/15	0.61	0.37	94,105,108,109	0
3	NAG	D	801	14/15	0.70	0.32	65,70,74,75	0
3	NAG	A	801	14/15	0.73	0.32	65,70,74,75	0
3	NAG	E	1512	14/15	0.73	0.25	94,105,108,109	0
3	NAG	C	800	14/15	0.75	0.24	76,81,84,85	0
3	NAG	G	1512	14/15	0.76	0.24	94,105,108,109	0
3	NAG	B	800	14/15	0.79	0.24	76,81,85,85	0
3	NAG	H	1486	14/15	0.79	0.28	86,104,108,109	0
3	NAG	E	1486	14/15	0.80	0.26	86,104,108,109	0
3	NAG	F	1486	14/15	0.83	0.23	86,104,108,109	0
3	NAG	D	800	14/15	0.89	0.22	76,81,85,85	0
3	NAG	G	1486	14/15	0.89	0.20	86,104,108,109	0
3	NAG	A	800	14/15	0.90	0.20	76,81,85,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.