W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2024 – 06:12 PM EST

PDB ID	:	8SIT
Title	:	Crystal structure of SARS-CoV-2 spike receptor-binding domain in complex with broadly neutralizing antibody CC84.24 Fab
Authors	:	Liu, H.; Wilson, I.A.
Deposited on	:	2023-04-16
Resolution	:	2.91 Å(reported)

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	:	2.36
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)	:	2.36

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 2.91 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.
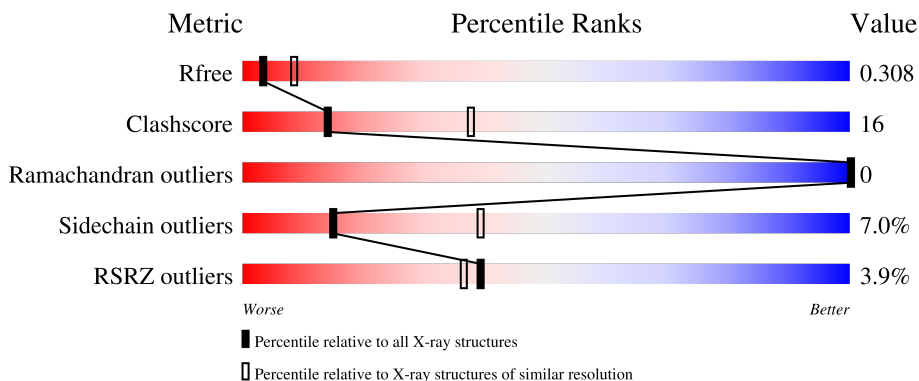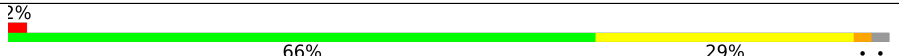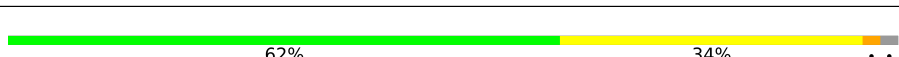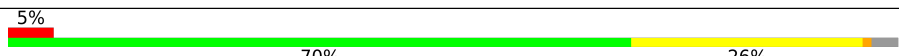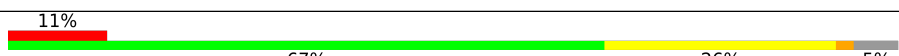
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 <=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	205	69% / 24% / • 5%
1	B	205	.% / 63% / 29% / • 5%
1	C	205	69% / 25% / • 5%
1	D	205	7% / 65% / 26% / • 7%
2	H	231	68% / 25% / • • •

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Mol	Chain	Length	Quality of chain
2	M	231	70% 28%
2	O	231	4% 60% 32%
2	Q	231	13% 59% 28% 8%
3	L	214	2% 66% 29%
3	N	214	62% 34%
3	P	214	5% 70% 26%
3	S	214	11% 67% 26% 5%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 18011 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	A	195	Total	C	N	O	S	0	0	0
			1508	966	251	283	8			
1	B	195	Total	C	N	O	S	0	0	0
			1484	950	245	281	8			
1	C	195	Total	C	N	O	S	0	0	0
			1508	969	250	281	8			
1	D	191	Total	C	N	O	S	0	0	0
			1329	838	230	253	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
A	537	HIS	-	expression tag	UNP P0DTC2
B	531	GLY	-	expression tag	UNP P0DTC2
B	532	HIS	-	expression tag	UNP P0DTC2
B	533	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
B	536	HIS	-	expression tag	UNP P0DTC2
B	537	HIS	-	expression tag	UNP P0DTC2
C	531	GLY	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2
C	537	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	531	GLY	-	expression tag	UNP P0DTC2
D	532	HIS	-	expression tag	UNP P0DTC2
D	533	HIS	-	expression tag	UNP P0DTC2
D	534	HIS	-	expression tag	UNP P0DTC2
D	535	HIS	-	expression tag	UNP P0DTC2
D	536	HIS	-	expression tag	UNP P0DTC2
D	537	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CC84.24 fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total 1618	C 1022	N 273	O 316	S 7	0	0	0
2	M	229	Total 1681	C 1060	N 285	O 329	S 7	0	0	0
2	O	224	Total 1611	C 1012	N 276	O 316	S 7	0	0	0
2	Q	212	Total 1414	C 884	N 246	O 279	S 5	0	0	0

- Molecule 3 is a protein called CC84.24 fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total 1508	C 944	N 254	O 306	S 4	0	0	0
3	N	209	Total 1520	C 950	N 255	O 311	S 4	0	0	0
3	P	208	Total 1439	C 901	N 243	O 291	S 4	0	0	0
3	S	204	Total 1363	C 849	N 234	O 276	S 4	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

Chain A:
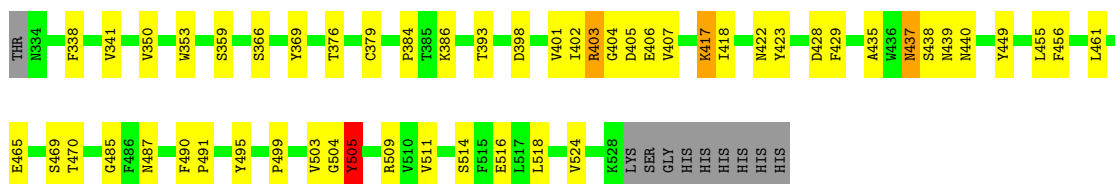
• Molecule 1: Spike protein S1

Chain B:

• Molecule 1: Spike protein S1

Chain C:

• Molecule 1: Spike protein S1

Chain D:

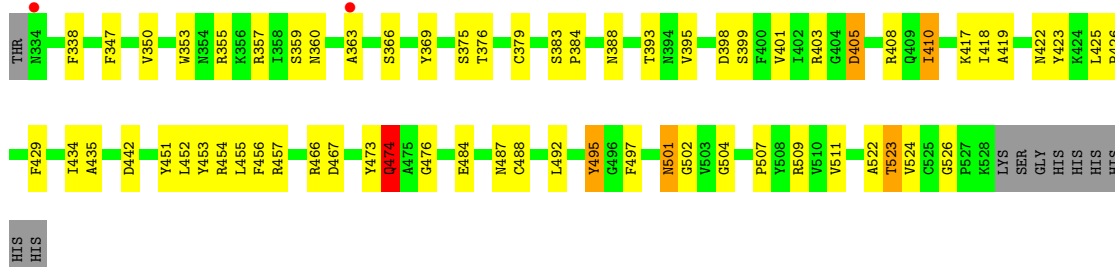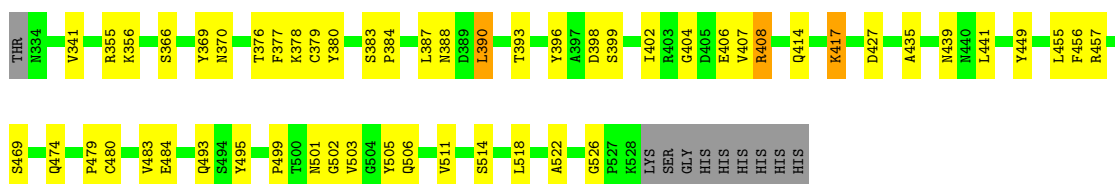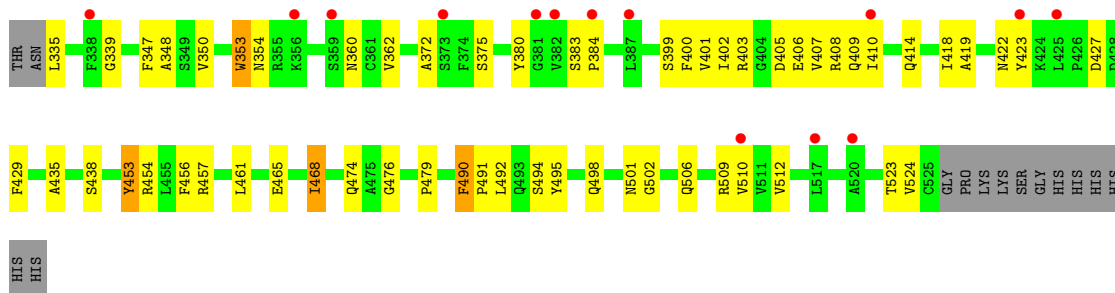THR ASN L335 F338 G339 F347 A348 S349 V350 W353 N354 R355 K356 S359 N360 C361 V362 A372 S373 F374 S375 Y380 G381 V382 S383 P384 L387 S399 F400 V401 I402 R403 G404 D405 E406 V407 R408 Q409 I410 Q414 I418 A419 N422 Y423 K424 L425 P426 D427 D428

F429 A435 S438 Y453 R454 L455 F456 R457 L461 E465 I468 Q474 A475 G476 P479 F490 P491 L492 S494 Y495 Q498 N501 G502 Q506 R509 V510 V511 V512 L517 A520 T523 V524 C525 GLY PRO LYS LYS SER GLY HIS HIS HIS HIS

HIS HIS

• Molecule 2: CC84.24 fab heavy chain

Chain H:

E1 V5 E6 L11 S17 A23 A24 F27 N35 Q39 L45 E46 W47 S50 I51 R52 Y56 I57 S58 Y59 A60 D61 S62 V63 R66 F67 M82 N82A S82B L82C D86 M87 Y91 R94 R97 D98 D100A Y100E F100K Q105

T110 K117 V121 F122 P123 L124 S128 LYS SER THR SER G133 G134 T135 Y145 F146 P147 E148 P149 V152 S153 W154 N155 L159 V163 V169 S173 Y176 S177 L178 V182 S188 LEU GLY THR Q192 I195 C196 N197 V198 N199 H200 N204 D208

K209 R210 P213 LYS SER CYS

• Molecule 2: CC84.24 fab heavy chain

Chain M:

E1 V2 Q3 L4 V5 E6 L11 V12 L18 R19 F27 M34 N35 Q39 A40 K43 W47 I51 R52 Y56 R66 F67 N73 A74 K75 N76 S77 L78 Q81 M82 L82C R83 A84 E85 D86 M87 Y91 C92 A95 G96 R97 Y100 D100A

Y100E Q100F R100G G100J F100K D101 Q106 T107 V111 P126 L138 K143 D144 P147 S153 W154 Q171 L175 Y176 S177 T193 Y194 I195 C196 N197 S203 N204 T205 K209 R210 V211 E212 P213 K214 SER CYS

• Molecule 2: CC84.24 fab heavy chain

Chain O:

E1 L4 V5 E6 G9 GLY L11 V12 L18 R19 C22 A23 A24 F27 S30 P31 Y32 S33 M34 N35 R38 Q39 A40 K43 G44 L45 E46 W47 V48 S49 S50 I51 R52 S52A S53 G54 S58 Y59 A60 V63 F67 T68 I69 S70 L78 Y79 R83

M87 A88 V89 Y90 Y91 C92 A93 R94 R97 Y100 D100A R100B Y100E G100J F100K D101 Y102 Q105 V109 T110 V111 S112 S113 T116 V121 L124 A125 P126 SER SER LYS SER T131 S132 G133 G134 T135 A136 A137 L138 G139 C140 D144 P147 E148 P149 V152

S156 L159 V163 H164 T165 F166 Q171 S172 L175 V182 T183 V184 P185 S186 Y194 N197 V198 N199 H200 K201 P202 S203 N204 T205 D208 V211 K214 SER CYS

• Molecule 2: CC84.24 fab heavy chain

Chain Q:

• Molecule 3: CC84.24 fab light chain

Chain L:

• Molecule 3: CC84.24 fab light chain

Chain N:

• Molecule 3: CC84.24 fab light chain

Chain P:

• Molecule 3: CC84.24 fab light chain

Chain S:

11%

67%　　　　　　　　　　　　　　26%　　　5%

GLN S2 T5 Q6 P7 V13 A19 R20 I21 T22 C23 G24 G25 I28 V33 Q34 W35 Y36 Q37 V47 V48 Y49 D50 D51 R54 P55 I58 R61 F62 N69 I75 S76 R77 V78 Y86 Y87 C88 Q89 V90 W91 D92 S93 D95A H95B W96 V97 F98

Q109 P110 K111 A112 A113 P114 S115 F119 L126 Q127 A128 ASN LYS ALA THR LEU V134 C135 L136 I137 F140 Y141 P142 V145 W149 K150 A151 S154 P155 V156 K157 A158 G159 V160 E161 T162 P165 S176 S177 Y178 L179 S180 L181 T182 Q185 W186 K187 S188 S193

C194 Q195 V196 T197 S201 T202 V203 E204 K205 T206 V207 A208 P209 THR GLU CYS SER

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.39Å 105.98Å 247.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.91 48.70 – 2.91	Depositor EDS
% Data completeness (in resolution range)	78.5 (48.70-2.91) 78.5 (48.70-2.91)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.261 , 0.309 0.261 , 0.308	Depositor DCC
R_{free} test set	2275 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å²)	55.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 30.0	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	18011	wwPDB-VP
Average B, all atoms (Å²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/1552	0.60	2/2117 (0.1%)
1	B	0.34	0/1527	0.56	2/2086 (0.1%)
1	C	0.28	0/1551	0.55	1/2114 (0.0%)
1	D	0.31	0/1363	0.57	1/1873 (0.1%)
2	H	0.40	2/1659 (0.1%)	0.79	8/2265 (0.4%)
2	M	0.27	0/1724	0.52	0/2355
2	O	0.44	1/1651 (0.1%)	0.73	3/2258 (0.1%)
2	Q	0.42	0/1447	0.64	2/1993 (0.1%)
3	L	0.33	0/1548	0.59	1/2130 (0.0%)
3	N	0.29	0/1560	0.54	0/2145
3	P	0.34	0/1477	0.57	0/2038
3	S	0.45	2/1399 (0.1%)	0.64	1/1932 (0.1%)
All	All	0.35	5/18458 (0.0%)	0.61	21/25306 (0.1%)

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	2
1	B	0	1
2	H	0	1
2	O	0	2
2	Q	0	1
3	L	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	163	VAL	CB-CG1	-6.55	1.39	1.52
3	S	176	SER	CB-OG	6.35	1.50	1.42
2	O	109	VAL	CB-CG1	-5.93	1.40	1.52
2	H	61	ASP	CG-OD1	5.85	1.38	1.25
3	S	78	VAL	CB-CG2	5.00	1.63	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	61	ASP	CB-CG-OD1	-13.44	106.20	118.30
2	H	159	LEU	CB-CG-CD2	-13.06	88.79	111.00
2	O	211	VAL	CG1-CB-CG2	9.37	125.89	110.90
2	O	109	VAL	CG1-CB-CG2	-8.31	97.60	110.90
1	A	505	TYR	N-CA-CB	-7.92	96.35	110.60

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	403	ARG	Sidechain
1	A	505	TYR	Sidechain
1	B	474	GLN	Sidechain
2	H	61	ASP	Sidechain
3	L	170	ASN	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	1508	0	1371	35	0
1	B	1484	0	1325	51	0
1	C	1508	0	1390	32	1
1	D	1329	0	1088	49	0
2	H	1618	0	1497	47	1
2	M	1681	0	1571	47	1
2	O	1611	0	1454	65	0
2	Q	1414	0	1177	61	0
3	L	1508	0	1387	48	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1520	0	1407	52	0
3	P	1439	0	1263	47	0
3	S	1363	0	1133	44	0
4	A	14	0	13	1	0
4	D	14	0	13	1	0
All	All	18011	0	16089	534	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 534 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)
3:S:193:SER:HB3	3:S:206:THR:HG23	1.33	1.10
3:S:193:SER:HB3	3:S:206:THR:CG2	1.83	1.07
1:B:474:GLN:NE2	1:B:476:GLY:O	1.93	1.00
2:H:123:PRO:HG3	2:H:209:LYS:HE3	1.50	0.93
2:M:6:GLU:OE2	2:M:92:CYS:N	2.02	0.92

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LEU:O	3:L:94:SER:OG[4_545]	2.16	0.04
2:H:173:SER:O	2:M:100(E):TYR:OH[4_445]	2.17	0.03

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	193/205 (94%)	191 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	193/205 (94%)	190 (98%)	3 (2%)	0	100	100
1	C	193/205 (94%)	189 (98%)	4 (2%)	0	100	100
1	D	189/205 (92%)	185 (98%)	4 (2%)	0	100	100
2	H	215/231 (93%)	209 (97%)	6 (3%)	0	100	100
2	M	227/231 (98%)	220 (97%)	7 (3%)	0	100	100
2	O	218/231 (94%)	213 (98%)	5 (2%)	0	100	100
2	Q	204/231 (88%)	196 (96%)	8 (4%)	0	100	100
3	L	208/214 (97%)	203 (98%)	5 (2%)	0	100	100
3	N	207/214 (97%)	205 (99%)	2 (1%)	0	100	100
3	P	206/214 (96%)	201 (98%)	5 (2%)	0	100	100
3	S	200/214 (94%)	193 (96%)	7 (4%)	0	100	100
All	All	2453/2600 (94%)	2395 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/177 (88%)	147 (95%)	8 (5%)	23	54
1	B	149/177 (84%)	144 (97%)	5 (3%)	37	69
1	C	156/177 (88%)	145 (93%)	11 (7%)	14	38
1	D	114/177 (64%)	106 (93%)	8 (7%)	15	39
2	H	168/193 (87%)	156 (93%)	12 (7%)	14	38
2	M	176/193 (91%)	172 (98%)	4 (2%)	50	79
2	O	161/193 (83%)	145 (90%)	16 (10%)	8	23
2	Q	124/193 (64%)	101 (82%)	23 (18%)	1	4
3	L	157/179 (88%)	144 (92%)	13 (8%)	11	30
3	N	162/179 (90%)	154 (95%)	8 (5%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	138/179 (77%)	132 (96%)	6 (4%)	29	61
3	S	120/179 (67%)	110 (92%)	10 (8%)	11	30
All	All	1780/2196 (81%)	1656 (93%)	124 (7%)	15	39

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	4	LEU
2	Q	179	SER
2	O	30	SER
2	Q	163	VAL
3	S	88	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	76	ASN
2	O	105	GLN
2	M	171	GLN
3	N	168	GLN
2	O	197	ASN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry ⓘ

2 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	#$|Z| > 2$
4	NAG	A	600	1	14,14,15	0.73	1 (7%)	17,19,21	1.30	2 (11%)
4	NAG	D	600	1	14,14,15	0.25	0	17,19,21	0.46	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
4	NAG	A	600	1	-	3/6/23/26	0/1/1/1
4	NAG	D	600	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	NAG	C1-C2	2.40	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	600	NAG	C2-N2-C7	4.07	128.70	122.90
4	A	600	NAG	C1-C2-N2	2.23	114.30	110.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	NAG	C8-C7-N2-C2
4	A	600	NAG	O7-C7-N2-C2
4	D	600	NAG	O5-C5-C6-O6
4	D	600	NAG	C3-C2-N2-C7
4	A	600	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	NAG	1	0
4	D	600	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	195/205 (95%)	-0.28	0	100 100	15, 31, 63, 91	0
1	B	195/205 (95%)	-0.11	2 (1%)	82 82	37, 63, 91, 116	0
1	C	195/205 (95%)	-0.23	0	100 100	22, 43, 79, 114	0
1	D	191/205 (93%)	0.36	14 (7%)	15 12	67, 93, 120, 139	0
2	H	221/231 (95%)	-0.10	1 (0%)	91 91	15, 44, 92, 123	0
2	M	229/231 (99%)	-0.22	0	100 100	25, 45, 79, 113	0
2	O	224/231 (96%)	0.19	10 (4%)	33 30	40, 80, 107, 145	0
2	Q	212/231 (91%)	0.68	30 (14%)	2 2	76, 103, 127, 154	0
3	L	210/214 (98%)	-0.13	5 (2%)	59 57	16, 51, 100, 137	0
3	N	209/214 (97%)	-0.22	1 (0%)	91 91	26, 45, 75, 90	0
3	P	208/214 (97%)	0.37	10 (4%)	30 27	49, 98, 126, 161	0
3	S	204/214 (95%)	0.54	24 (11%)	4 3	64, 98, 127, 148	0
All	All	2493/2600 (95%)	0.07	97 (3%)	39 36	15, 66, 117, 161	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	53	SER	5.9
3	S	201	SER	5.0
3	S	202	THR	4.9
1	D	381	GLY	4.7
2	Q	120	SER	4.7

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 monosaccharides 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
4	NAG	D	600	14/15	0.85	0.16	84,90,94,95	0
4	NAG	A	600	14/15	0.91	0.16	36,41,49,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.