



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:48 AM UTC

PDB ID : 8I5H / pdb_00008i5h
Title : Crystal structure of SARS-CoV-2 delta variant spike receptor-binding domain (RBD) in complex with NCV2SG48 Fab
Authors : Yamamoto, A.; Higashiura, A.
Deposited on : 2023-01-25
Resolution : 2.38 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)
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

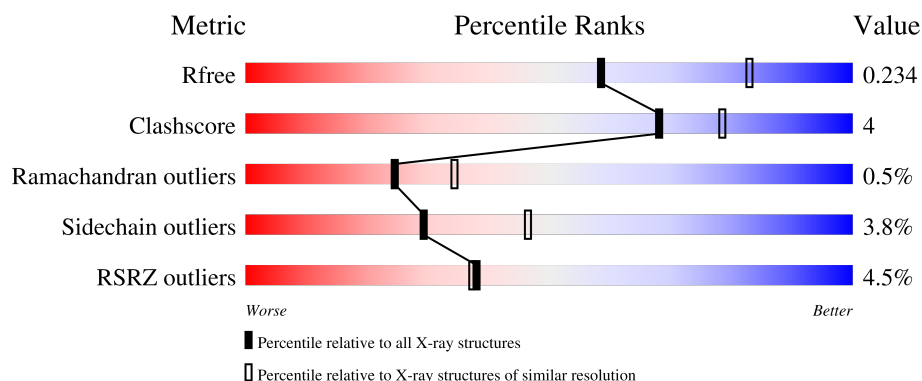
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	A	194	14% 85% 15% .
1	D	194	9% 84% 15% .
1	R	194	7% 87% 12% .
2	B	230	2% 79% 12% 8%
2	E	230	2% 83% 7% 8%

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Mol	Chain	Length	Quality of chain
2	H	230	2% 87% 7%
3	C	215	3% 88% 10%
3	F	215	% 89% 9%
3	L	215	% 89% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14631 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	R	194	Total	C	N	O	S	0	1	0
			1549	992	263	286	8			
1	A	194	Total	C	N	O	S	0	1	0
			1549	992	263	286	8			
1	D	194	Total	C	N	O	S	0	0	0
			1541	987	260	286	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	452	ARG	LEU	variant	UNP P0DTC2
R	478	LYS	THR	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1594	1009	269	310	6			
2	B	211	Total	C	N	O	S	0	0	0
			1584	1004	267	307	6			
2	E	211	Total	C	N	O	S	0	0	0
			1586	1005	267	308	6			

- Molecule 3 is a protein called Fab Light chain.

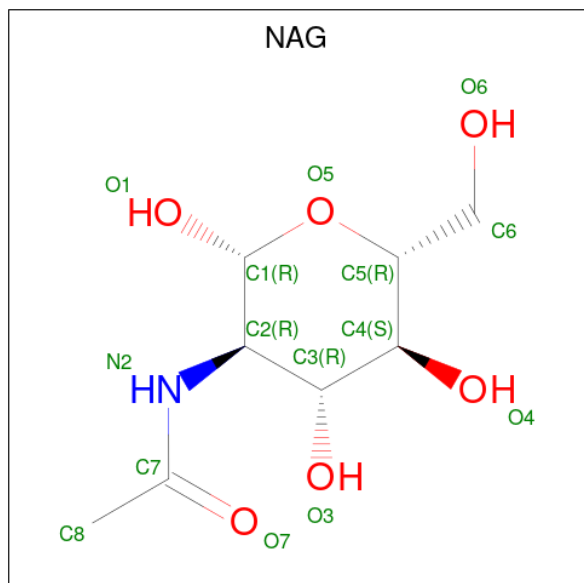
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1630	1019	279	328	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1630	1019	279	328	4			
3	F	214	Total	C	N	O	S	0	0	0
			1630	1019	279	328	4			

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	36	Total	O	0	0
			36	36		
5	H	44	Total	O	0	0
			44	44		
5	L	32	Total	O	0	0
			32	32		
5	A	18	Total	O	0	0
			18	18		

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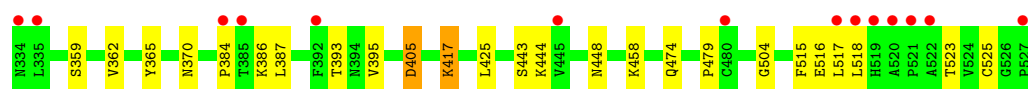
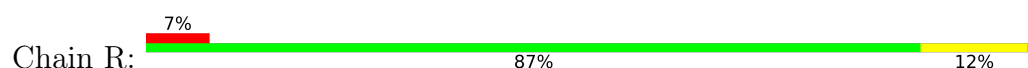
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	32	Total 32	O 32	0	0
5	C	41	Total 41	O 41	0	0
5	D	16	Total 16	O 16	0	0
5	E	35	Total 35	O 35	0	0
5	F	42	Total 42	O 42	0	0

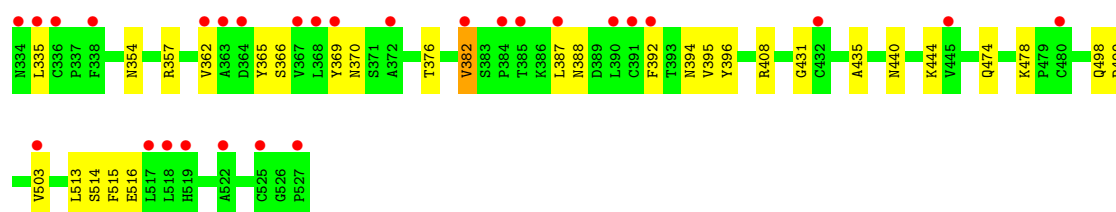
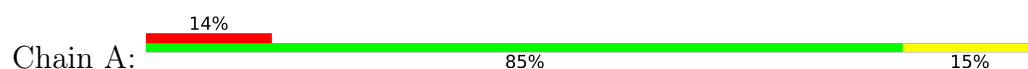
3 Residue-property plots [i](#)

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.

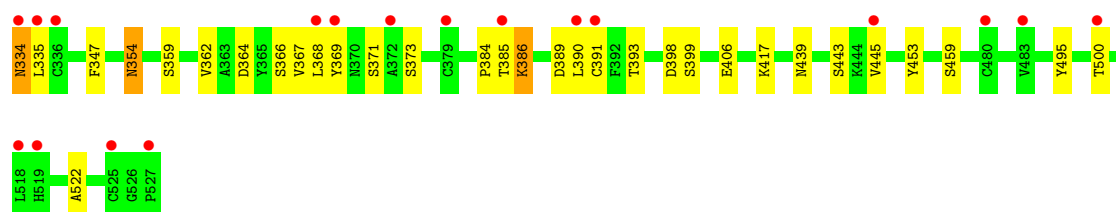
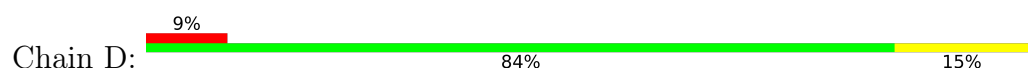
- Molecule 1: Spike protein S1



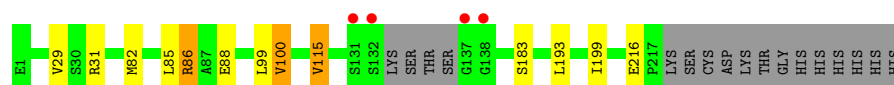
- Molecule 1: Spike protein S1



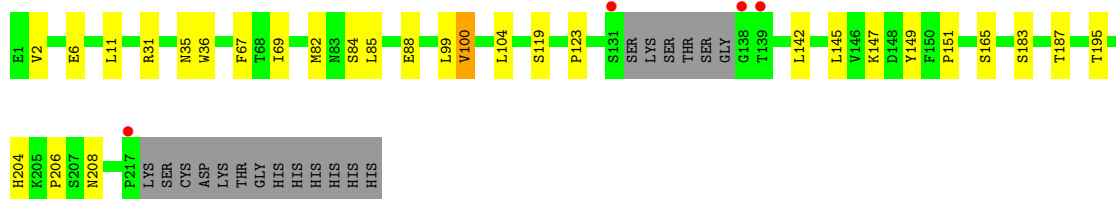
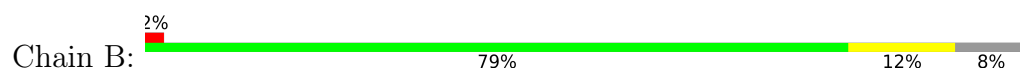
- Molecule 1: Spike protein S1



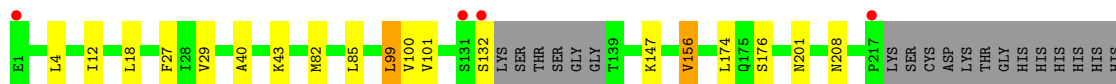
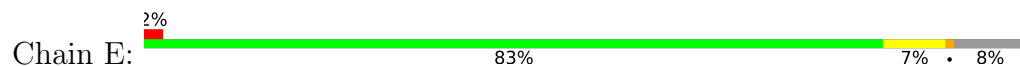
- Molecule 2: Fab Heavy chain



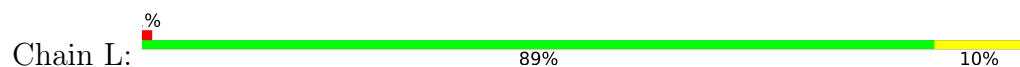
- Molecule 2: Fab Heavy chain



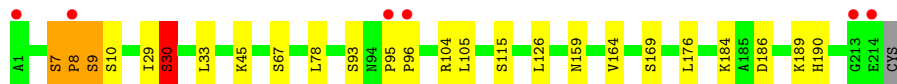
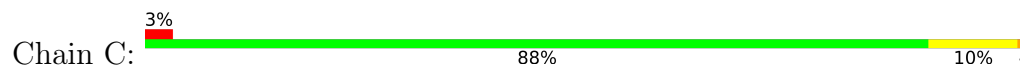
- Molecule 2: Fab Heavy chain



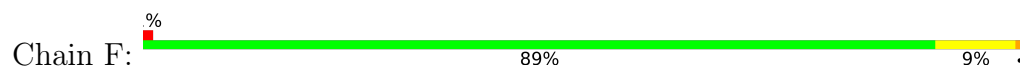
- Molecule 3: Fab Light chain



- Molecule 3: Fab Light chain



- Molecule 3: Fab Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.81Å 113.73Å 272.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.98 – 2.38 42.98 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.98-2.38) 99.9 (42.98-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.188 , 0.230 0.192 , 0.234	Depositor DCC
R_{free} test set	5534 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14631	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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	0.29	0/1596	0.45	0/2169
1	D	0.31	0/1585	0.48	0/2155
1	R	0.37	0/1596	0.56	0/2169
2	B	0.33	0/1620	0.54	0/2208
2	E	0.35	0/1622	0.61	2/2211 (0.1%)
2	H	0.36	0/1630	0.59	0/2221
3	C	0.34	0/1665	0.61	3/2262 (0.1%)
3	F	0.39	0/1665	0.60	1/2262 (0.0%)
3	L	0.37	0/1665	0.61	2/2262 (0.1%)
All	All	0.35	0/14644	0.57	8/19919 (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
2	B	0	1
2	E	0	1
2	H	0	1
3	C	0	2
3	F	0	2
3	L	0	1
All	All	0	8

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	SER	CA-C-N	-7.10	109.95	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
3	C	7	SER	C-N-CA	-7.10	109.95	127.00
3	C	7	SER	C-N-CD	6.93	135.85	120.60
3	L	29	ILE	CA-C-N	5.92	132.85	121.54
3	L	29	ILE	C-N-CA	5.92	132.85	121.54
2	E	174	LEU	CA-C-N	-5.75	110.56	121.54
2	E	174	LEU	C-N-CA	-5.75	110.56	121.54
3	F	21	ILE	N-CA-C	5.10	119.94	109.34

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	99	LEU	Peptide
3	C	29	ILE	Peptide
3	C	95	PRO	Peptide
2	E	99	LEU	Peptide
3	F	21	ILE	Peptide
3	F	29	ILE	Peptide
2	H	99	LEU	Peptide
3	L	95	PRO	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	1549	0	1473	21	0
1	D	1541	0	1460	16	0
1	R	1549	0	1473	13	0
2	B	1584	0	1561	12	0
2	E	1586	0	1563	6	0
2	H	1594	0	1569	8	0
3	C	1630	0	1597	12	0
3	F	1630	0	1597	11	0
3	L	1630	0	1597	10	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
4	R	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	0	1	0
5	B	32	0	0	0	0
5	C	41	0	0	2	0
5	D	16	0	0	0	0
5	E	35	0	0	0	0
5	F	42	0	0	1	0
5	H	44	0	0	0	0
5	L	32	0	0	0	0
5	R	36	0	0	0	0
All	All	14631	0	13929	101	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 4.

All (101) 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:L:22:THR:HG22	3:L:72:THR:HG22	1.63	0.80
3:C:190:HIS:ND1	5:C:301:HOH:O	2.15	0.79
3:F:138:ASN:OD1	3:F:139:ASN:ND2	2.20	0.74
3:L:104:ARG:NH1	3:L:106:GLU:OE1	2.25	0.68
1:R:393:THR:HG21	1:R:518:LEU:HB2	1.77	0.67
3:C:7:SER:HA	3:C:8:PRO:O	1.97	0.64
1:D:334:ASN:HD22	1:D:334:ASN:N	1.95	0.62
3:C:45:LYS:NZ	5:C:302:HOH:O	2.32	0.62
3:L:24:ARG:NH1	3:L:25:ALA:O	2.32	0.62
3:F:21:ILE:HD11	3:F:73:LEU:HD23	1.82	0.61
2:B:145:LEU:HD22	2:B:147:LYS:HB2	1.84	0.60
3:F:45:LYS:NZ	5:F:303:HOH:O	2.35	0.59
3:F:155:LEU:HD12	3:F:155:LEU:H	1.67	0.59
1:A:366:SER:HA	1:A:369:TYR:CE1	2.38	0.59
1:A:357:ARG:HG3	1:A:396:TYR:HE1	1.68	0.59
1:D:439:ASN:O	1:D:443:SER:HB3	2.06	0.56
1:A:382:VAL:HG11	1:A:387:LEU:HD13	1.87	0.56
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.88	0.56
1:A:365:TYR:H	1:A:388:ASN:HD21	1.54	0.55
2:H:86:ARG:O	2:H:115:VAL:HG11	2.07	0.55
1:D:335:LEU:HD13	1:D:362:VAL:HG13	1.88	0.54
1:R:365:TYR:CD2	1:R:387:LEU:HB3	2.43	0.54
1:A:408:ARG:NH1	5:A:701:HOH:O	2.42	0.53
2:B:82:MET:HB3	2:B:85:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:VAL:HG11	3:C:93:SER:HA	1.91	0.52
1:A:357:ARG:HG3	1:A:396:TYR:CE1	2.44	0.52
2:E:82:MET:HE2	2:E:85:LEU:HD21	1.91	0.52
2:H:86:ARG:HB2	2:H:88:GLU:OE1	2.11	0.51
2:H:82:MET:HE2	2:H:85:LEU:HD21	1.91	0.50
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.94	0.50
2:E:4:LEU:HD21	2:E:27:PHE:HZ	1.76	0.50
1:A:335:LEU:HD23	1:A:362:VAL:HG13	1.93	0.50
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.76	0.49
1:R:405:ASP:HB3	1:R:504:GLY:O	2.12	0.49
3:L:146:LYS:HB3	3:L:198:THR:HB	1.94	0.49
3:F:155:LEU:H	3:F:155:LEU:CD1	2.26	0.49
1:A:498:GLN:NE2	3:C:30:SER:HB3	2.27	0.49
1:R:458:LYS:HE2	2:H:31:ARG:HH22	1.77	0.48
1:R:384:PRO:C	1:R:386:LYS:H	2.21	0.48
1:D:384:PRO:C	1:D:386:LYS:H	2.21	0.48
2:E:40:ALA:HB3	2:E:43:LYS:HD3	1.95	0.48
3:C:159:ASN:OD1	3:C:159:ASN:N	2.47	0.48
1:D:369:TYR:HD2	1:D:385:THR:HG23	1.78	0.48
1:A:376:THR:HB	1:A:435:ALA:HB3	1.96	0.48
1:D:371:SER:OG	1:D:373:SER:OG	2.31	0.47
3:F:155:LEU:HD12	3:F:155:LEU:N	2.30	0.47
1:A:392:PHE:HB3	1:A:516:GLU:O	2.15	0.47
1:A:444:LYS:O	1:A:499:PRO:HD3	2.14	0.47
3:C:186:ASP:O	3:C:189:LYS:HG2	2.15	0.47
1:R:393:THR:O	1:R:523:THR:HG22	2.15	0.46
2:B:11:LEU:HB2	2:B:151:PRO:HG3	1.96	0.46
3:F:151:VAL:HG23	3:F:156:GLN:HG3	1.98	0.46
1:A:365:TYR:CD2	1:A:387:LEU:HG	2.51	0.46
1:R:474:GLN:OE1	1:R:479:PRO:HA	2.16	0.45
2:H:88:GLU:H	2:H:88:GLU:CD	2.23	0.45
1:R:444:LYS:HB2	1:R:448:ASN:HB2	1.98	0.45
2:E:99:LEU:O	2:E:101:VAL:N	2.49	0.45
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.82	0.45
1:A:474:GLN:O	2:B:31:ARG:NH1	2.49	0.45
2:H:193:LEU:HD23	2:H:193:LEU:HA	1.84	0.45
1:D:367:VAL:HG13	1:D:368:LEU:HG	1.98	0.45
3:F:22:THR:HA	3:F:71:PHE:O	2.17	0.45
1:D:391:CYS:HB3	1:D:522:ALA:HB1	2.00	0.44
1:D:364:ASP:OD2	1:D:366:SER:OG	2.35	0.44
1:D:390:LEU:HD23	1:D:390:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:PRO:O	1:D:385:THR:OG1	2.26	0.44
3:C:10:SER:HA	3:C:104:ARG:O	2.17	0.44
1:R:395:VAL:HG22	1:R:515:PHE:HD1	1.82	0.44
1:R:516:GLU:HG2	1:R:518:LEU:HG	2.00	0.44
2:B:204:HIS:CD2	2:B:206:PRO:HD2	2.53	0.43
3:C:126:LEU:O	3:C:184:LYS:HD2	2.17	0.43
3:L:42:LYS:HE3	3:L:42:LYS:HB3	1.81	0.43
1:R:425:LEU:HA	1:R:425:LEU:HD23	1.78	0.43
3:C:164:VAL:HG22	3:C:176:LEU:HD12	1.99	0.43
3:F:125:GLN:HG2	3:F:130:THR:O	2.18	0.43
1:A:382:VAL:CG1	1:A:387:LEU:HD13	2.48	0.43
2:B:35:ASN:HD22	2:B:104:LEU:HD11	1.83	0.43
1:D:417:LYS:HD2	1:D:453:TYR:CE1	2.54	0.42
2:B:85:LEU:HD23	2:B:85:LEU:HA	1.84	0.42
2:B:100:VAL:CG1	3:C:93:SER:HA	2.49	0.42
1:D:347:PHE:CE2	1:D:399:SER:HB2	2.54	0.42
2:H:100:VAL:CG1	3:L:93:SER:HA	2.50	0.42
2:H:100:VAL:HG11	3:L:93:SER:HA	2.01	0.42
2:E:156:VAL:HA	2:E:201:ASN:O	2.19	0.42
1:R:362:VAL:HA	1:R:525:CYS:O	2.20	0.42
1:A:440:ASN:OD1	1:A:440:ASN:N	2.53	0.42
1:R:417:LYS:HE2	3:L:93:SER:HB2	2.01	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.83	0.41
2:E:12:ILE:HD12	2:E:18:LEU:HD13	2.03	0.41
1:A:394:ASN:HB2	1:A:516:GLU:OE1	2.21	0.41
1:A:365:TYR:CE2	1:A:387:LEU:HG	2.56	0.41
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.55	0.41
3:C:78:LEU:HD11	3:C:105:LEU:HD21	2.03	0.41
1:D:406:GLU:OE1	1:D:495:TYR:OH	2.30	0.41
2:B:123:PRO:HB3	2:B:149:TYR:HB3	2.02	0.40
3:F:186:ASP:HA	3:F:189:LYS:HE2	2.03	0.40
1:D:354:ASN:O	1:D:398:ASP:HA	2.21	0.40
2:B:67:PHE:CZ	2:B:82:MET:HE3	2.56	0.40
3:L:78:LEU:HD11	3:L:105:LEU:HD11	2.04	0.40
2:B:36:TRP:HD1	2:B:69:ILE:HD12	1.86	0.40
1:D:369:TYR:CD2	1:D:384:PRO:HB2	2.56	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	A	193/194 (100%)	182 (94%)	11 (6%)	0	100	100
1	D	192/194 (99%)	182 (95%)	10 (5%)	0	100	100
1	R	193/194 (100%)	183 (95%)	10 (5%)	0	100	100
2	B	207/230 (90%)	203 (98%)	3 (1%)	1 (0%)	24	34
2	E	207/230 (90%)	199 (96%)	7 (3%)	1 (0%)	24	34
2	H	209/230 (91%)	206 (99%)	2 (1%)	1 (0%)	24	34
3	C	212/215 (99%)	200 (94%)	8 (4%)	4 (2%)	6	7
3	F	212/215 (99%)	201 (95%)	10 (5%)	1 (0%)	24	34
3	L	212/215 (99%)	203 (96%)	8 (4%)	1 (0%)	24	34
All	All	1837/1917 (96%)	1759 (96%)	69 (4%)	9 (0%)	24	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	8	PRO
2	H	100	VAL
2	B	100	VAL
2	E	100	VAL
3	L	96	PRO
3	C	96	PRO
3	F	22	THR
3	C	30	SER
3	C	9	SER

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	168/167 (101%)	163 (97%)	5 (3%)	36	56
1	D	167/167 (100%)	158 (95%)	9 (5%)	20	32
1	R	168/167 (101%)	162 (96%)	6 (4%)	31	49
2	B	176/193 (91%)	165 (94%)	11 (6%)	16	26
2	E	177/193 (92%)	171 (97%)	6 (3%)	32	51
2	H	177/193 (92%)	171 (97%)	6 (3%)	32	51
3	C	186/187 (100%)	180 (97%)	6 (3%)	34	53
3	F	186/187 (100%)	180 (97%)	6 (3%)	34	53
3	L	186/187 (100%)	181 (97%)	5 (3%)	39	59
All	All	1591/1641 (97%)	1531 (96%)	60 (4%)	29	46

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	359	SER
1	R	370	ASN
1	R	405	ASP
1	R	417	LYS
1	R	443	SER
1	R	517	LEU
2	H	29	VAL
2	H	86	ARG
2	H	115	VAL
2	H	183	SER
2	H	199	ILE
2	H	216	GLU
3	L	30	SER
3	L	33	LEU
3	L	39	LYS
3	L	67	SER
3	L	77	SER
1	A	354	ASN
1	A	370	ASN
1	A	382	VAL
1	A	503	VAL
1	A	514	SER
2	B	2	VAL

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Mol	Chain	Res	Type
2	B	6	GLU
2	B	84	SER
2	B	88	GLU
2	B	119	SER
2	B	142	LEU
2	B	165	SER
2	B	183	SER
2	B	187	THR
2	B	195	THR
2	B	208	ASN
3	C	9	SER
3	C	30	SER
3	C	33	LEU
3	C	67	SER
3	C	115	SER
3	C	169	SER
1	D	334	ASN
1	D	354	ASN
1	D	359	SER
1	D	386	LYS
1	D	389	ASP
1	D	393	THR
1	D	445	VAL
1	D	459	SER
1	D	500	THR
2	E	29	VAL
2	E	132	SER
2	E	147	LYS
2	E	156	VAL
2	E	176	SER
2	E	208	ASN
3	F	12	SER
3	F	30	SER
3	F	54	LEU
3	F	56	SER
3	F	106	GLU
3	F	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN

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Mol	Chain	Res	Type
2	H	81	GLN
2	H	83	ASN
2	H	196	GLN
3	L	38	GLN
3	L	161	GLN
2	B	39	GLN
3	C	38	GLN
3	C	190	HIS
1	D	394	ASN
2	E	168	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	R	601	1	14,14,15	0.44	0	17,19,21	0.50	0
4	NAG	D	601	1	14,14,15	0.45	0	17,19,21	0.87	1 (5%)
4	NAG	A	601	1	14,14,15	0.78	1 (7%)	17,19,21	0.83	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
4	NAG	R	601	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	2.39	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	NAG	C1-O5-C5	3.24	116.52	112.19
4	A	601	NAG	C1-O5-C5	2.90	116.07	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	601	NAG	C4-C5-C6-O6
4	D	601	NAG	O5-C5-C6-O6
4	R	601	NAG	C8-C7-N2-C2
4	R	601	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	194/194 (100%)	0.85	28 (14%) 6 5	30, 66, 108, 117	1 (0%)
1	D	194/194 (100%)	0.61	18 (9%) 14 13	45, 61, 87, 105	0
1	R	194/194 (100%)	0.51	14 (7%) 21 20	24, 55, 86, 111	1 (0%)
2	B	211/230 (91%)	0.43	4 (1%) 66 65	46, 57, 79, 96	0
2	E	211/230 (91%)	0.16	4 (1%) 66 65	41, 53, 70, 96	0
2	H	213/230 (92%)	0.02	4 (1%) 66 65	39, 50, 65, 94	0
3	C	214/215 (99%)	0.28	6 (2%) 55 54	42, 56, 75, 88	0
3	F	214/215 (99%)	0.08	2 (0%) 81 80	40, 50, 64, 81	0
3	L	214/215 (99%)	0.24	3 (1%) 73 72	41, 54, 69, 79	0
All	All	1859/1917 (96%)	0.34	83 (4%) 38 37	24, 55, 85, 117	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	138	GLY	4.7
3	C	1	ALA	4.6
2	H	137	GLY	4.2
1	A	372	ALA	4.2
1	D	385	THR	4.2
1	A	527	PRO	3.8
2	H	132	SER	3.7
1	R	517	LEU	3.6
1	A	503	VAL	3.5
3	F	1	ALA	3.5
2	E	132	SER	3.5
1	R	445	VAL	3.5
1	A	519	HIS	3.4
1	A	367	VAL	3.4
1	A	335	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	131	SER	3.3
1	A	385	THR	3.2
3	C	96	PRO	3.1
1	A	369	TYR	3.0
2	B	139	THR	2.9
3	L	214	GLU	2.9
1	D	391	CYS	2.9
1	D	335	LEU	2.9
1	A	445	VAL	2.8
1	A	368	LEU	2.8
1	A	390	LEU	2.8
1	A	338	PHE	2.8
1	R	385	THR	2.8
3	C	95	PRO	2.8
1	A	362	VAL	2.8
1	R	384	PRO	2.7
1	A	432	CYS	2.7
1	D	483	VAL	2.7
1	A	517	LEU	2.7
1	R	335	LEU	2.7
2	E	1	GLU	2.6
1	A	525	CYS	2.6
1	R	527	PRO	2.6
1	D	369	TYR	2.6
1	R	518	LEU	2.6
1	A	363	ALA	2.5
1	D	372	ALA	2.5
2	B	217	PRO	2.5
1	A	334	ASN	2.5
1	R	519	HIS	2.5
1	A	392	PHE	2.5
1	A	518	LEU	2.5
1	R	521	PRO	2.5
1	D	379	CYS	2.5
1	D	518	LEU	2.5
1	A	391	CYS	2.4
1	D	445	VAL	2.4
1	A	387	LEU	2.4
1	A	384	PRO	2.4
3	F	21	ILE	2.4
3	L	30	SER	2.4
1	D	390	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	L	1	ALA	2.3
1	D	480	CYS	2.3
1	R	334	ASN	2.3
3	C	8	PRO	2.3
3	C	214	GLU	2.3
1	D	334	ASN	2.3
1	D	519	HIS	2.3
1	A	382	VAL	2.3
1	A	364	ASP	2.2
2	E	217	PRO	2.2
1	R	480	CYS	2.2
1	D	527	PRO	2.2
1	A	336	CYS	2.2
2	E	131	SER	2.2
1	D	336	CYS	2.1
1	D	368	LEU	2.1
2	H	138	GLY	2.1
3	C	213	GLY	2.1
1	D	500	THR	2.1
2	H	131	SER	2.1
1	R	520	ALA	2.0
1	R	392	PHE	2.0
1	R	522	ALA	2.0
1	A	522	ALA	2.0
1	A	480	CYS	2.0
1	D	525	CYS	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($\text{\AA}^2$)	Q<0.9
4	NAG	R	601	14/15	0.72	0.15	72,84,96,96	0
4	NAG	A	601	14/15	0.77	0.15	92,97,100,100	0
4	NAG	D	601	14/15	0.83	0.13	74,87,96,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.