



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:28 PM UTC

PDB ID : 8RJ7 / pdb_00008rj7
Title : The crystal structure of the SARS-CoV-2 receptor binding domain in complex with the neutralizing nanobody 1.29
Authors : Casasnovas, J.M.; Fernandez, L.A.; Silva, K.
Deposited on : 2023-12-20
Resolution : 2.10 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

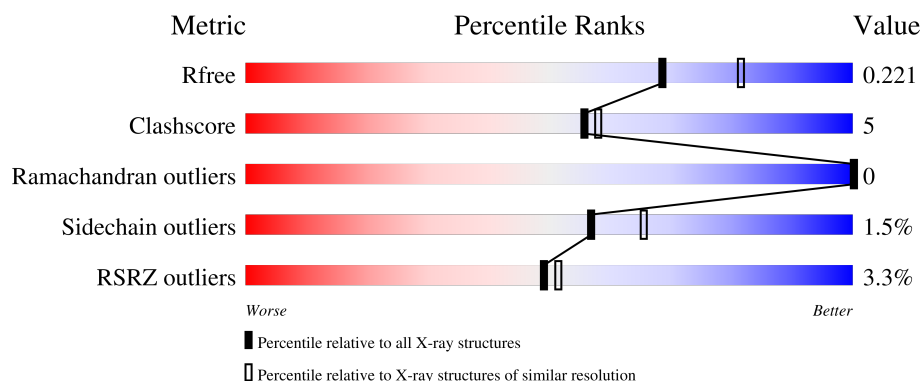
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	203	0% 86% 10% •
1	C	203	0% 85% 12% •
1	E	203	2% 85% 10% •
1	G	203	0% 83% 10% 6%
1	I	203	4% 84% 10% • 5%

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Mol	Chain	Length	Quality of chain
2	B	126	5% 83% 13%
2	D	126	5% 90% 7%
2	F	126	5% 87% 8% 5%
2	H	126	4% 85% 10% 5%
2	J	126	6% 85% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13135 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	196	Total	C	N	O	S	0	0	0
			1546	992	257	289	8			
1	C	197	Total	C	N	O	S	0	0	0
			1557	998	260	291	8			
1	E	195	Total	C	N	O	S	0	0	0
			1542	990	257	287	8			
1	G	190	Total	C	N	O	S	0	0	0
			1511	970	252	283	6			
1	I	192	Total	C	N	O	S	0	0	0
			1515	974	251	282	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	GLY	-	expression tag	UNP P0DTC2
A	331	SER	-	expression tag	UNP P0DTC2
A	529	LEU	-	expression tag	UNP P0DTC2
A	530	VAL	-	expression tag	UNP P0DTC2
A	531	PRO	-	expression tag	UNP P0DTC2
A	532	ARG	-	expression tag	UNP P0DTC2
C	330	GLY	-	expression tag	UNP P0DTC2
C	331	SER	-	expression tag	UNP P0DTC2
C	529	LEU	-	expression tag	UNP P0DTC2
C	530	VAL	-	expression tag	UNP P0DTC2
C	531	PRO	-	expression tag	UNP P0DTC2
C	532	ARG	-	expression tag	UNP P0DTC2
E	330	GLY	-	expression tag	UNP P0DTC2
E	331	SER	-	expression tag	UNP P0DTC2
E	529	LEU	-	expression tag	UNP P0DTC2
E	530	VAL	-	expression tag	UNP P0DTC2
E	531	PRO	-	expression tag	UNP P0DTC2
E	532	ARG	-	expression tag	UNP P0DTC2
G	330	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	331	SER	-	expression tag	UNP P0DTC2
G	529	LEU	-	expression tag	UNP P0DTC2
G	530	VAL	-	expression tag	UNP P0DTC2
G	531	PRO	-	expression tag	UNP P0DTC2
G	532	ARG	-	expression tag	UNP P0DTC2
I	330	GLY	-	expression tag	UNP P0DTC2
I	331	SER	-	expression tag	UNP P0DTC2
I	529	LEU	-	expression tag	UNP P0DTC2
I	530	VAL	-	expression tag	UNP P0DTC2
I	531	PRO	-	expression tag	UNP P0DTC2
I	532	ARG	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Camel-derived nanobody 1.29.

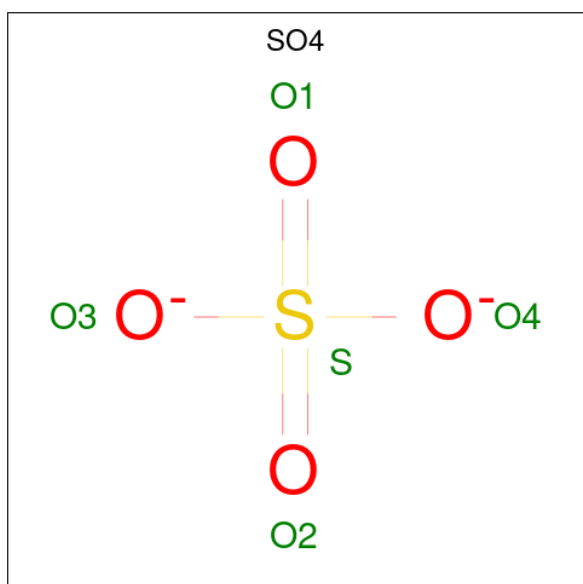
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			897	555	154	185	3			
2	D	122	Total	C	N	O	S	0	0	0
			899	554	156	186	3			
2	F	120	Total	C	N	O	S	0	0	0
			893	553	154	183	3			
2	H	120	Total	C	N	O	S	0	0	0
			892	552	153	184	3			
2	J	121	Total	C	N	O	S	0	0	0
			892	553	154	182	3			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



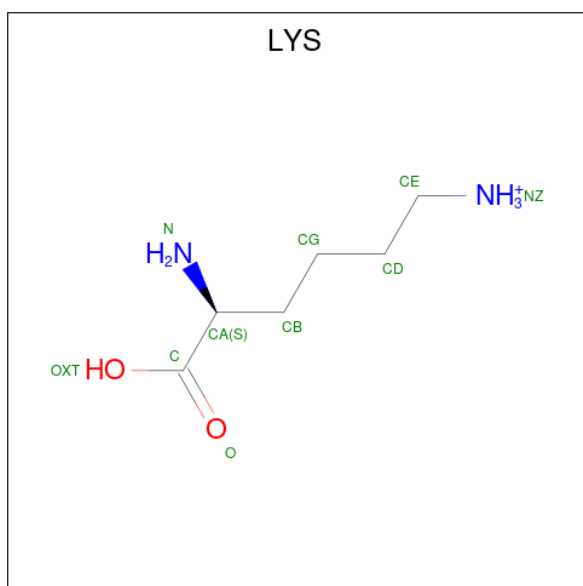
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	14	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

- Molecule 5 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 9 6 2 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0
6	C	120	Total O 120 120	0	0
6	E	88	Total O 88 88	0	0
6	G	168	Total O 168 168	0	0

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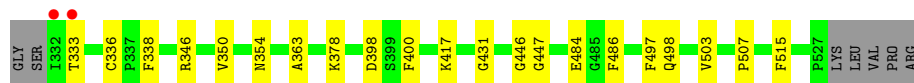
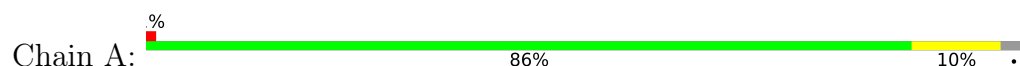
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	83	Total 83	O 83	0	0
6	D	68	Total 68	O 68	0	0
6	F	44	Total 44	O 44	0	0
6	H	69	Total 69	O 69	0	0
6	I	67	Total 67	O 67	0	0
6	J	39	Total 39	O 39	0	0

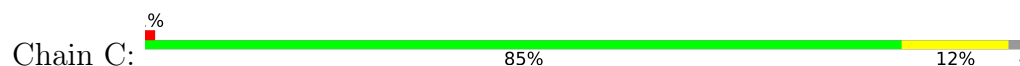
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

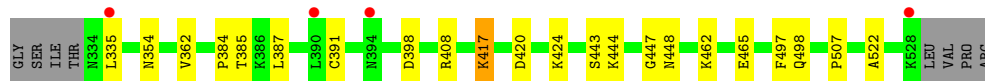
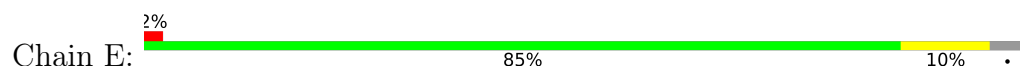
- Molecule 1: Spike protein S1



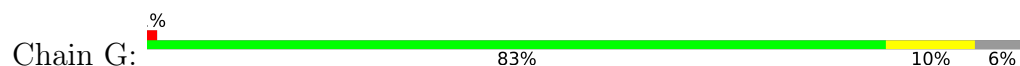
- Molecule 1: Spike protein S1



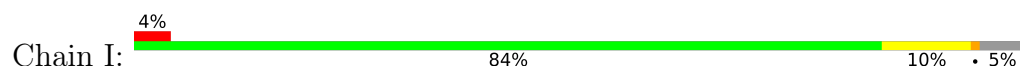
- Molecule 1: Spike protein S1

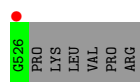


- Molecule 1: Spike protein S1

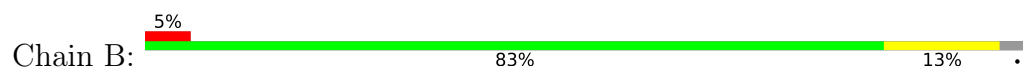


- Molecule 1: Spike protein S1

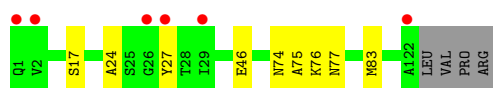
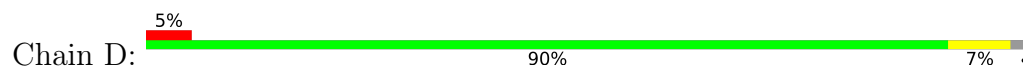




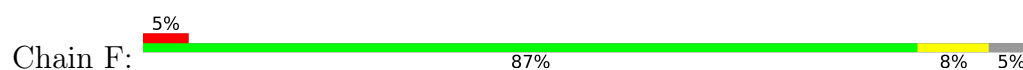
- Molecule 2: Camel-derived nanobody 1.29



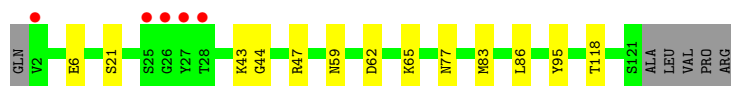
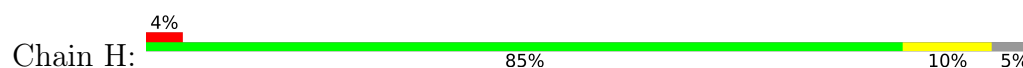
- Molecule 2: Camel-derived nanobody 1.29



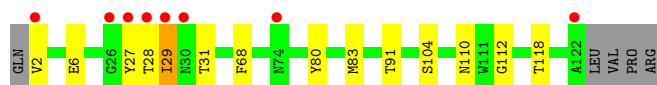
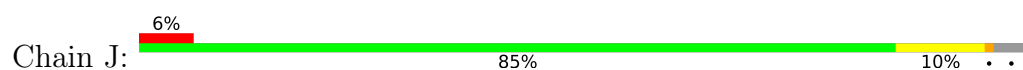
- Molecule 2: Camel-derived nanobody 1.29



- Molecule 2: Camel-derived nanobody 1.29



- Molecule 2: Camel-derived nanobody 1.29



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	89.16Å 89.16Å 200.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.52 – 2.10 43.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.52-2.10) 99.4 (43.52-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.181 , 0.222 0.181 , 0.221	Depositor DCC
R_{free} test set	5184 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l 0.029 for h,-h-k,-l 0.013 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13135	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: SO4, 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	0.34	0/1590	0.49	0/2165
1	C	0.35	0/1601	0.52	0/2179
1	E	0.30	0/1586	0.50	0/2158
1	G	0.38	0/1554	0.52	0/2115
1	I	0.28	0/1558	0.44	0/2120
2	B	0.36	0/914	0.52	0/1241
2	D	0.35	0/915	0.51	0/1242
2	F	0.31	0/910	0.53	0/1235
2	H	0.36	0/909	0.48	0/1234
2	J	0.30	0/909	0.48	0/1235
All	All	0.33	0/12446	0.50	0/16924

There are no bond length outliers.

There are no bond angle outliers.

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	A	1546	0	1459	16	0
1	C	1557	0	1475	18	0
1	E	1542	0	1461	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1511	0	1427	15	0
1	I	1515	0	1431	15	0
2	B	897	0	838	9	0
2	D	899	0	842	8	0
2	F	893	0	834	8	0
2	H	892	0	833	8	0
2	J	892	0	831	7	0
3	A	14	0	13	0	0
3	C	14	0	13	4	0
3	E	14	0	13	0	0
3	G	14	0	13	0	0
3	I	14	0	13	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	H	5	0	0	0	0
5	C	9	0	12	0	0
6	A	141	0	0	6	0
6	B	83	0	0	0	1
6	C	120	0	0	6	0
6	D	68	0	0	2	0
6	E	88	0	0	2	0
6	F	44	0	0	2	0
6	G	168	0	0	7	1
6	H	69	0	0	2	0
6	I	67	0	0	5	0
6	J	39	0	0	1	0
All	All	13135	0	11508	112	1

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 5.

All (112) 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:C:383:SER:HB3	1:C:386:LYS:HE2	1.38	1.06
1:C:408:ARG:NH1	6:C:703:HOH:O	2.02	0.91
1:G:466:ARG:NH2	6:G:702:HOH:O	2.04	0.90
1:I:484:GLU:OE1	6:I:701:HOH:O	1.92	0.85
1:C:364:ASP:OD1	6:C:701:HOH:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:496:GLY:O	6:G:701:HOH:O	1.96	0.84
1:C:496:GLY:O	6:C:702:HOH:O	1.96	0.81
2:D:46:GLU:OE2	6:D:301:HOH:O	2.00	0.80
2:F:47:ARG:HH11	2:F:47:ARG:HG2	1.50	0.76
1:G:523:THR:O	6:G:703:HOH:O	2.06	0.73
2:B:83:MET:HE2	2:B:86:LEU:HD21	1.70	0.72
1:A:446:GLY:O	6:A:701:HOH:O	2.09	0.69
1:I:496:GLY:O	6:I:702:HOH:O	2.10	0.69
2:H:118:THR:OG1	6:H:301:HOH:O	2.09	0.69
2:H:83:MET:HE2	2:H:86:LEU:HD21	1.75	0.68
1:G:473:TYR:OH	6:G:704:HOH:O	2.11	0.67
1:I:417:LYS:HD3	1:I:455:LEU:HD12	1.77	0.67
1:G:357:ARG:HD2	1:G:394:ASN:HD21	1.59	0.66
1:A:498:GLN:NE2	6:A:701:HOH:O	2.29	0.66
2:H:77:ASN:OD1	6:H:302:HOH:O	2.15	0.65
1:E:444:LYS:HG2	1:E:448:ASN:HB2	1.78	0.64
1:E:391:CYS:HB3	1:E:522:ALA:HB1	1.83	0.61
2:B:28:THR:OG1	2:B:30:ASN:ND2	2.35	0.60
2:B:31:THR:HG22	2:B:53:THR:HG21	1.84	0.59
1:E:420:ASP:OD1	6:E:701:HOH:O	2.17	0.59
2:F:113:GLN:NE2	6:F:201:HOH:O	2.34	0.59
1:C:366:SER:N	6:C:701:HOH:O	2.37	0.57
1:I:366:SER:OG	6:I:704:HOH:O	2.18	0.56
2:D:27:TYR:HA	2:D:77:ASN:HD21	1.70	0.56
2:F:83:MET:HE2	2:F:86:LEU:HD21	1.87	0.56
2:F:84:ASN:ND2	6:F:202:HOH:O	2.37	0.56
1:E:443:SER:O	1:E:444:LYS:HD3	2.06	0.55
1:A:447:GLY:HA2	1:A:498:GLN:HG2	1.88	0.55
1:G:339:GLY:O	1:G:343:ASN:HB2	2.07	0.55
2:H:62:ASP:HA	2:H:65:LYS:HG3	1.89	0.55
1:I:379:CYS:O	2:J:104:SER:HB3	2.06	0.54
1:I:408:ARG:NH2	6:I:706:HOH:O	2.38	0.54
1:I:408:ARG:NH2	2:J:110:ASN:OD1	2.41	0.53
2:B:40:ALA:HB3	2:B:43:LYS:HE2	1.91	0.53
1:A:378:LYS:NZ	6:A:706:HOH:O	2.42	0.53
1:I:408:ARG:NE	6:I:706:HOH:O	2.27	0.51
1:C:461:LEU:HD22	1:C:465:GLU:HG2	1.91	0.51
1:I:384:PRO:HA	1:I:387:LEU:HD12	1.93	0.51
2:B:2:VAL:HG13	2:B:110:ASN:ND2	2.26	0.51
1:C:368:LEU:HD21	3:C:602:NAG:H83	1.93	0.50
1:E:462:LYS:HG2	1:E:465:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:379:CYS:HB3	1:I:382:VAL:HG13	1.92	0.50
1:C:367:VAL:N	6:C:701:HOH:O	2.07	0.50
1:C:394:ASN:HB3	1:C:516:GLU:HB3	1.95	0.48
1:C:447:GLY:HA2	1:C:498:GLN:HG3	1.94	0.48
2:H:47:ARG:NH2	2:H:59:ASN:OD1	2.47	0.48
1:A:484:GLU:HB2	6:A:743:HOH:O	2.14	0.48
1:E:408:ARG:NH2	2:F:109:ASN:O	2.47	0.48
1:I:357:ARG:HG3	1:I:396:TYR:CE1	2.49	0.47
2:J:80:TYR:OH	6:J:201:HOH:O	2.07	0.47
2:J:68:PHE:CZ	2:J:83:MET:HG2	2.49	0.47
1:I:443:SER:O	1:I:444:LYS:HD3	2.14	0.47
1:G:393:THR:CG2	1:G:518:LEU:HB2	2.46	0.46
2:D:24:ALA:HB3	2:D:77:ASN:OD1	2.15	0.46
1:E:424:LYS:NZ	6:E:706:HOH:O	2.35	0.46
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.55	0.46
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.97	0.46
1:A:486:PHE:HD2	6:A:810:HOH:O	1.99	0.46
1:C:343:ASN:HD21	3:C:602:NAG:C1	2.29	0.46
1:G:358:ILE:O	6:G:705:HOH:O	2.20	0.46
1:G:357:ARG:HH11	1:G:394:ASN:ND2	2.13	0.45
2:B:6:GLU:HA	2:B:21:SER:O	2.16	0.45
1:A:417:LYS:HD3	1:A:417:LYS:HA	1.46	0.45
6:G:704:HOH:O	2:D:75:ALA:HB3	2.16	0.45
1:I:393:THR:HG21	1:I:518:LEU:HB2	1.99	0.45
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.52	0.45
1:E:335:LEU:HD12	1:E:362:VAL:O	2.16	0.45
1:A:417:LYS:HB2	6:A:725:HOH:O	2.17	0.45
1:C:343:ASN:HD21	3:C:602:NAG:H2	1.81	0.44
2:D:74:ASN:ND2	6:D:305:HOH:O	2.49	0.44
1:C:444:LYS:HD2	1:C:448:ASN:HB2	2.00	0.44
1:G:424:LYS:HD3	6:G:764:HOH:O	2.17	0.44
1:C:339:GLY:O	1:C:343:ASN:HB2	2.18	0.44
1:I:390:LEU:HD23	1:I:392:PHE:CZ	2.53	0.44
2:J:91:THR:HG23	2:J:118:THR:HA	1.99	0.44
1:E:354:ASN:O	1:E:398:ASP:HA	2.18	0.43
1:A:338:PHE:CE2	1:A:363:ALA:HB1	2.53	0.43
1:C:365:TYR:CD2	1:C:387:LEU:HB3	2.53	0.43
1:G:462:LYS:HE3	1:G:465:GLU:OE1	2.19	0.43
2:H:6:GLU:HA	2:H:21:SER:O	2.18	0.43
1:I:387:LEU:HD11	1:I:432:CYS:SG	2.58	0.43
2:D:27:TYR:HA	2:D:77:ASN:ND2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:6:GLU:OE2	2:J:112:GLY:HA3	2.19	0.42
1:A:503:VAL:HG21	2:B:95:TYR:CG	2.54	0.42
1:G:503:VAL:HG21	2:H:95:TYR:CG	2.54	0.42
1:E:443:SER:C	1:E:444:LYS:HD3	2.44	0.42
2:F:47:ARG:HG2	2:F:47:ARG:NH1	2.24	0.42
1:C:471:GLU:N	6:C:710:HOH:O	2.46	0.42
1:E:384:PRO:HA	1:E:387:LEU:HD12	2.02	0.42
2:J:29:ILE:C	2:J:31:THR:H	2.28	0.42
1:E:417:LYS:HA	1:E:417:LYS:HE3	2.02	0.42
2:D:17:SER:HA	2:D:83:MET:O	2.19	0.42
1:C:332:ILE:HG13	1:C:333:THR:H	1.85	0.41
1:C:343:ASN:ND2	3:C:602:NAG:H2	2.35	0.41
2:B:18:LEU:HD21	2:B:117:VAL:HG13	2.02	0.41
2:H:43:LYS:HG2	2:H:44:GLY:O	2.19	0.41
1:E:497:PHE:CE2	1:E:507:PRO:HB3	2.55	0.41
2:F:107:ASP:OD2	2:F:109:ASN:ND2	2.54	0.41
1:A:354:ASN:O	1:A:398:ASP:HA	2.19	0.41
1:A:486:PHE:CD1	2:F:57:ASN:HA	2.56	0.41
1:G:395:VAL:HG22	1:G:515:PHE:HD1	1.85	0.41
1:A:497:PHE:CE2	1:A:507:PRO:HB3	2.57	0.41
1:E:447:GLY:HA2	1:E:498:GLN:HG2	2.02	0.40
2:D:76:LYS:HA	2:D:76:LYS:HD3	1.89	0.40
1:G:354:ASN:O	1:G:398:ASP:HA	2.22	0.40
2:B:113:GLN:HG2	2:B:114:GLY:N	2.37	0.40
1:G:386:LYS:HE3	1:G:386:LYS:HB3	1.60	0.40

All (1) 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)
6:G:852:HOH:O	6:B:365:HOH:O[3_455]	1.91	0.29

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	194/203 (96%)	187 (96%)	7 (4%)	0	100	100
1	C	195/203 (96%)	186 (95%)	9 (5%)	0	100	100
1	E	193/203 (95%)	183 (95%)	10 (5%)	0	100	100
1	G	188/203 (93%)	183 (97%)	5 (3%)	0	100	100
1	I	190/203 (94%)	182 (96%)	8 (4%)	0	100	100
2	B	119/126 (94%)	116 (98%)	3 (2%)	0	100	100
2	D	120/126 (95%)	119 (99%)	1 (1%)	0	100	100
2	F	118/126 (94%)	117 (99%)	1 (1%)	0	100	100
2	H	118/126 (94%)	117 (99%)	1 (1%)	0	100	100
2	J	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
All	All	1554/1645 (94%)	1507 (97%)	47 (3%)	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	167/175 (95%)	165 (99%)	2 (1%)	63	72
1	C	169/175 (97%)	167 (99%)	2 (1%)	63	72
1	E	167/175 (95%)	165 (99%)	2 (1%)	63	72
1	G	163/175 (93%)	162 (99%)	1 (1%)	78	86
1	I	163/175 (93%)	158 (97%)	5 (3%)	35	39
2	B	92/97 (95%)	92 (100%)	0	100	100
2	D	92/97 (95%)	92 (100%)	0	100	100
2	F	91/97 (94%)	89 (98%)	2 (2%)	45	53
2	H	92/97 (95%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	90/97 (93%)	86 (96%)	4 (4%)	25	26
All	All	1286/1360 (95%)	1268 (99%)	18 (1%)	57	67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	THR
1	A	346	ARG
1	C	335	LEU
1	C	417	LYS
1	E	385	THR
1	E	417	LYS
1	G	472	ILE
2	F	1	GLN
2	F	50	VAL
1	I	371	SER
1	I	390	LEU
1	I	417	LYS
1	I	477	SER
1	I	514	SER
2	J	2	VAL
2	J	27	TYR
2	J	28	THR
2	J	29	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	C	343	ASN
1	E	354	ASN
1	E	440	ASN
1	E	498	GLN
1	G	394	ASN
1	G	493	GLN
1	G	519	HIS
2	B	30	ASN
2	B	82	GLN
2	B	84	ASN
2	D	30	ASN
2	D	59	ASN

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Mol	Chain	Res	Type
2	D	82	GLN
2	D	84	ASN
2	F	113	GLN
2	H	57	ASN
2	H	82	GLN
1	I	450	ASN
2	J	13	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	C	602	-	14,14,15	0.35	0	17,19,21	0.65	0
4	SO4	E	602	-	4,4,4	0.23	0	6,6,6	0.25	0
5	LYS	C	601	-	7,8,9	0.54	0	3,8,10	0.34	0
4	SO4	H	201	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	B	201	-	4,4,4	0.31	0	6,6,6	0.20	0
3	NAG	A	601	1	14,14,15	0.34	0	17,19,21	0.38	0
4	SO4	A	602	-	4,4,4	0.25	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	601	1	14,14,15	0.43	0	17,19,21	0.53	0
3	NAG	G	601	1	14,14,15	0.64	0	17,19,21	0.65	0
4	SO4	D	201	-	4,4,4	0.16	0	6,6,6	0.26	0
3	NAG	I	601	1	14,14,15	0.28	0	17,19,21	0.44	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	C	602	-	-	0/6/23/26	0/1/1/1
5	LYS	C	601	-	-	4/6/7/9	-
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	E	601	1	-	2/6/23/26	0/1/1/1
3	NAG	G	601	1	-	2/6/23/26	0/1/1/1
3	NAG	I	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	LYS	N-CA-CB-CG
5	C	601	LYS	C-CA-CB-CG
3	A	601	NAG	O5-C5-C6-O6
3	I	601	NAG	O5-C5-C6-O6
3	I	601	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	E	601	NAG	C4-C5-C6-O6
5	C	601	LYS	CA-CB-CG-CD
3	G	601	NAG	O5-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
5	C	601	LYS	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	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	A	196/203 (96%)	-0.03	2 (1%) 79 81	26, 39, 55, 79	0
1	C	197/203 (97%)	-0.00	3 (1%) 72 74	25, 39, 55, 72	0
1	E	195/203 (96%)	0.30	4 (2%) 63 66	32, 45, 69, 80	0
1	G	190/203 (93%)	-0.15	3 (1%) 70 73	24, 33, 55, 83	0
1	I	192/203 (94%)	0.55	9 (4%) 36 38	31, 52, 72, 78	0
2	B	121/126 (96%)	-0.07	6 (4%) 34 36	25, 33, 58, 97	0
2	D	122/126 (96%)	-0.01	6 (4%) 35 37	25, 35, 61, 87	0
2	F	120/126 (95%)	0.29	6 (5%) 34 36	32, 43, 79, 103	1 (0%)
2	H	120/126 (95%)	0.02	5 (4%) 40 42	26, 38, 57, 65	0
2	J	121/126 (96%)	0.13	8 (6%) 24 26	30, 42, 66, 84	1 (0%)
All	All	1574/1645 (95%)	0.11	52 (3%) 49 51	24, 40, 67, 103	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	122	ALA	5.3
2	B	27	TYR	4.5
2	D	27	TYR	4.4
2	F	27	TYR	4.3
2	H	27	TYR	4.1
2	J	122	ALA	4.1
2	D	122	ALA	3.8
1	I	335	LEU	3.6
2	B	2	VAL	3.4
1	G	391	CYS	3.3
2	H	2	VAL	3.3
1	C	332	ILE	3.2
2	J	27	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	29	ILE	3.1
2	F	29	ILE	3.1
1	I	522	ALA	3.1
1	E	335	LEU	3.1
2	H	26	GLY	2.9
2	D	1	GLN	2.9
1	G	335	LEU	2.8
2	H	25	SER	2.8
1	I	381	GLY	2.8
1	E	394	ASN	2.8
1	G	523	THR	2.8
2	B	26	GLY	2.7
1	I	521	PRO	2.7
2	F	2	VAL	2.7
2	D	2	VAL	2.6
2	J	26	GLY	2.6
2	J	2	VAL	2.6
1	I	481	ASN	2.5
2	D	26	GLY	2.5
2	J	29	ILE	2.5
1	I	526	GLY	2.4
2	B	30	ASN	2.4
1	A	333	THR	2.4
2	F	31	THR	2.4
1	A	332	ILE	2.4
1	E	528	LYS	2.3
2	H	28	THR	2.3
1	E	390	LEU	2.3
2	B	29	ILE	2.2
2	J	28	THR	2.2
1	C	372	ALA	2.1
1	I	517	LEU	2.1
2	F	28	THR	2.1
2	J	74	ASN	2.1
2	F	101	TYR	2.1
1	I	363	ALA	2.1
1	I	341	VAL	2.0
2	J	30	ASN	2.0
1	C	528	LYS	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
5	LYS	C	601	9/10	0.72	0.19	67,77,82,90	0
3	NAG	E	601	14/15	0.80	0.09	62,74,78,79	0
3	NAG	C	602	14/15	0.80	0.12	57,70,74,82	0
3	NAG	A	601	14/15	0.86	0.09	60,67,73,75	0
3	NAG	I	601	14/15	-	-	65,70,72,73	14
3	NAG	G	601	14/15	0.91	0.08	41,45,47,48	0
4	SO4	A	602	5/5	0.97	0.06	38,39,41,45	0
4	SO4	B	201	5/5	0.98	0.05	33,38,39,40	0
4	SO4	H	201	5/5	0.98	0.07	36,45,47,47	0
4	SO4	E	602	5/5	0.98	0.04	34,36,40,42	0
4	SO4	D	201	5/5	0.99	0.04	31,33,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.