



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:26 PM UTC

PDB ID : 8GPY / pdb_00008gpy
Title : Crystal structure of Omicron BA.4/5 RBD in complex with a neutralizing antibody scFv
Authors : Gao, Y.X.; Song, Z.D.; Wang, W.M.; Guo, Y.
Deposited on : 2022-08-27
Resolution : 2.51 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
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

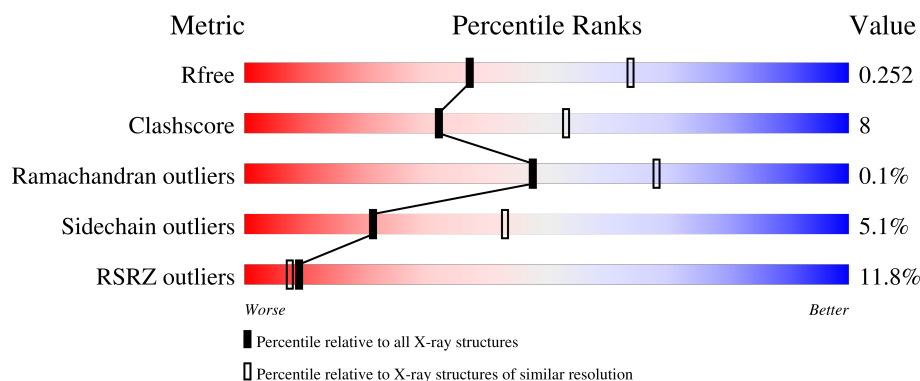
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	201	21% 77% 16% • 5%
1	B	201	22% 66% 22% • 10%
2	C	232	% 84% 13% •
2	E	232	3% 82% 16% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6558 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	191	Total	C	N	O	S	0	0	0
			1524	982	258	276	8			
1	B	180	Total	C	N	O	S	0	0	0
			1458	940	245	265	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	531	ALA	-	expression tag	UNP P0DTC2
A	532	ALA	-	expression tag	UNP P0DTC2
A	533	ALA	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	531	ALA	-	expression tag	UNP P0DTC2
B	532	ALA	-	expression tag	UNP P0DTC2
B	533	ALA	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called scFv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	227	Total	C	N	O	S	27	0	0
			1704	1068	286	341	9			
2	E	230	Total	C	N	O	S	24	0	0
			1723	1079	290	345	9			

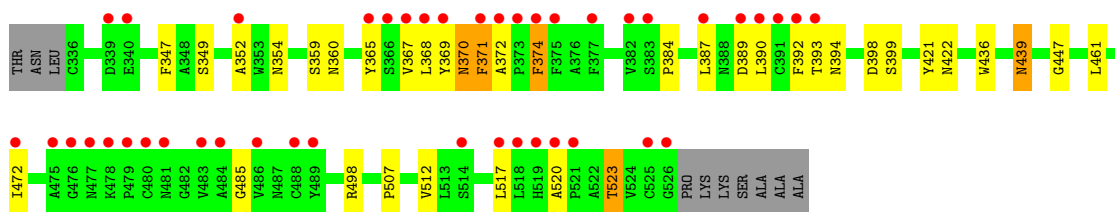
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	11	Total	O	0	0
			11	11		
3	C	53	Total	O	0	0
			53	53		
3	E	69	Total	O	0	0
			69	69		

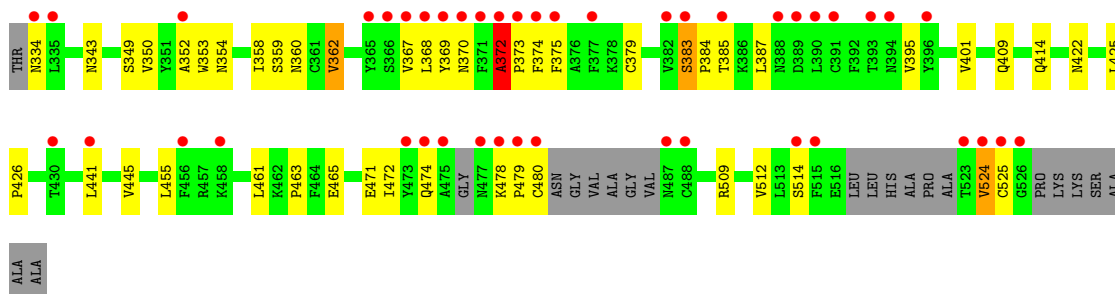
3 Residue-property plots [i](#)

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.

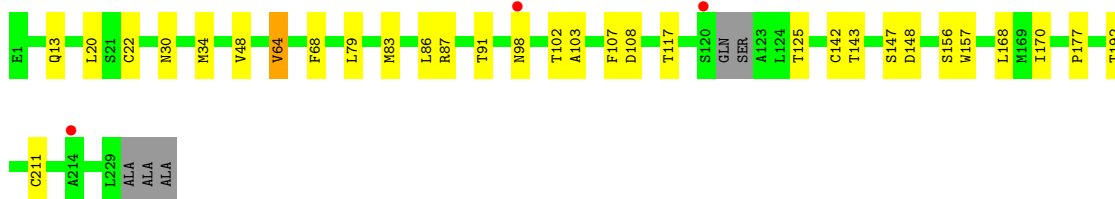
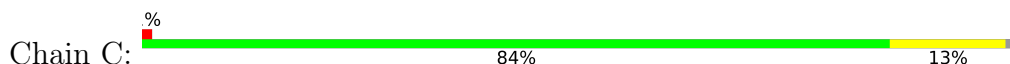
- Molecule 1: Spike protein S1



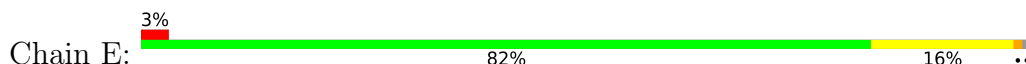
- Molecule 1: Spike protein S1

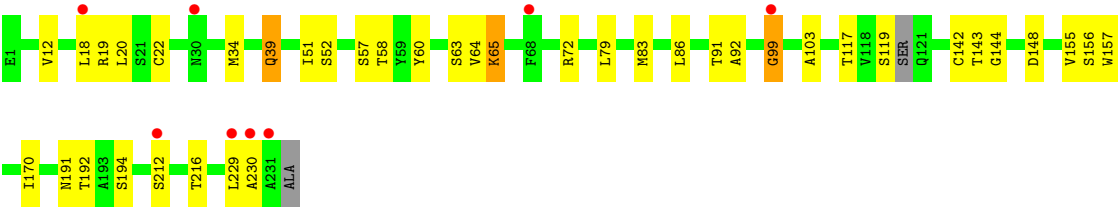


- Molecule 2: scFv



- Molecule 2: scFv





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.86Å 92.09Å 89.27Å 90.00° 92.40° 90.00°	Depositor
Resolution (Å)	49.60 – 2.51 49.60 – 2.51	Depositor EDS
% Data completeness (in resolution range)	71.8 (49.60-2.51) 81.9 (49.60-2.51)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.251 0.217 , 0.252	Depositor DCC
R_{free} test set	2003 reflections (5.84%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/1570	0.58	6/2136 (0.3%)
1	B	0.33	0/1499	0.61	6/2033 (0.3%)
2	C	0.27	0/1744	0.54	3/2370 (0.1%)
2	E	0.45	0/1763	0.62	4/2396 (0.2%)
All	All	0.34	0/6576	0.59	19/8935 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	48	VAL	N-CA-C	8.70	119.30	111.81
1	B	367	VAL	N-CA-C	-8.30	104.94	112.90
1	A	372	ALA	N-CA-C	7.61	120.42	109.84
1	A	374	PHE	N-CA-C	7.34	121.34	110.48
2	C	48	VAL	CB-CA-C	-7.06	103.43	111.55
1	A	422	ASN	N-CA-C	6.83	121.77	112.68
2	E	230	ALA	N-CA-C	5.68	117.62	110.24
1	B	372	ALA	CA-C-N	-5.64	113.89	119.92
1	B	372	ALA	C-N-CA	-5.64	113.89	119.92
2	C	108	ASP	N-CA-C	-5.39	107.36	114.31
1	B	353	TRP	N-CA-C	-5.27	101.69	110.17
1	A	439	ASN	N-CA-C	5.27	118.49	111.75
1	B	374	PHE	N-CA-C	5.20	117.00	110.91
2	E	39	GLN	N-CA-C	-5.17	99.67	108.26
1	A	369	TYR	N-CA-C	-5.16	105.73	112.23
2	E	39	GLN	CB-CA-C	5.14	118.06	110.14
1	A	485	GLY	N-CA-C	5.05	116.87	110.20
2	E	99	GLY	N-CA-C	-5.04	101.24	113.18
1	B	368	LEU	N-CA-C	-5.01	102.11	109.62

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	1524	0	1448	42	0
1	B	1458	0	1376	23	0
2	C	1704	0	1615	19	0
2	E	1723	0	1633	16	0
3	A	16	0	0	0	0
3	B	11	0	0	1	0
3	C	53	0	0	2	0
3	E	69	0	0	0	0
All	All	6558	0	6072	99	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 8.

All (99) 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:A:387:LEU:HA	1:A:390:LEU:HD21	1.22	1.16
1:A:387:LEU:HA	1:A:390:LEU:CD2	1.82	1.10
1:A:387:LEU:CD2	1:A:390:LEU:HD21	1.87	1.04
1:A:387:LEU:HD23	1:A:390:LEU:CD2	1.87	1.03
1:A:390:LEU:HB3	1:A:392:PHE:CD2	1.95	1.02
1:A:387:LEU:HD23	1:A:390:LEU:HD21	1.41	0.99
1:A:387:LEU:CA	1:A:390:LEU:HD21	1.97	0.94
1:A:387:LEU:CD2	1:A:390:LEU:CD2	2.49	0.89
1:A:390:LEU:HB3	1:A:392:PHE:CE2	2.08	0.88
1:A:390:LEU:HD22	1:A:392:PHE:HE2	1.38	0.86
2:C:34:MET:SD	2:C:98:ASN:ND2	2.53	0.82
1:A:384:PRO:HA	1:A:387:LEU:HG	1.67	0.77
1:A:360:ASN:H	1:A:523:THR:HG22	1.51	0.76
1:A:390:LEU:HB3	1:A:392:PHE:HD2	1.52	0.73
1:A:393:THR:CG2	1:A:520:ALA:O	2.38	0.72
1:A:390:LEU:HD22	1:A:392:PHE:CE2	2.25	0.69
2:C:156:SER:HB3	2:C:211:CYS:HB3	1.75	0.69
1:A:390:LEU:CD2	1:A:392:PHE:HE2	2.09	0.66
2:C:157:TRP:HB2	2:C:170:ILE:HB	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLN:HG3	1:B:480:CYS:HB2	1.81	0.63
2:E:39:GLN:O	2:E:92:ALA:HB1	2.00	0.62
1:A:393:THR:HG21	1:A:520:ALA:O	2.00	0.61
1:A:387:LEU:HD22	1:A:390:LEU:HD21	1.81	0.61
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.83	0.61
1:B:369:TYR:CD2	1:B:370:ASN:N	2.70	0.60
1:A:387:LEU:HD22	1:A:390:LEU:CD2	2.33	0.59
1:A:393:THR:HG22	1:A:520:ALA:O	2.01	0.59
1:B:354:ASN:ND2	3:B:601:HOH:O	2.36	0.59
1:A:389:ASP:OD1	1:A:389:ASP:N	2.36	0.59
2:C:142:CYS:O	2:C:192:THR:HA	2.03	0.58
2:C:87:ARG:NH1	3:C:305:HOH:O	2.36	0.58
1:B:409:GLN:HA	1:B:414:GLN:HG2	1.87	0.55
1:A:387:LEU:CD2	1:A:390:LEU:HD22	2.35	0.55
2:C:13:GLN:NE2	3:C:303:HOH:O	2.31	0.55
1:A:354:ASN:OD1	1:B:360:ASN:ND2	2.40	0.55
1:A:387:LEU:HA	1:A:390:LEU:HD23	1.83	0.54
2:C:83:MET:HB3	2:C:86:LEU:HD21	1.89	0.54
2:C:91:THR:HG23	2:C:117:THR:HA	1.89	0.54
2:E:157:TRP:HB2	2:E:170:ILE:HB	1.90	0.54
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.90	0.54
1:A:387:LEU:CB	1:A:390:LEU:HD21	2.37	0.53
1:A:387:LEU:HD23	1:A:390:LEU:HD22	1.87	0.52
1:B:384:PRO:O	1:B:387:LEU:HB2	2.09	0.52
1:A:447:GLY:HA2	1:A:498:ARG:HG2	1.93	0.51
1:B:358:ILE:HB	1:B:395:VAL:HB	1.93	0.50
1:B:425:LEU:HD21	1:B:512:VAL:HG11	1.92	0.50
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.94	0.49
1:A:368:LEU:HA	1:A:371:PHE:HB2	1.94	0.49
1:A:390:LEU:CB	1:A:392:PHE:CE2	2.90	0.49
1:A:398:ASP:HB2	1:A:512:VAL:HB	1.94	0.49
1:A:387:LEU:CA	1:A:390:LEU:CD2	2.70	0.49
1:B:478:LYS:O	1:B:479:PRO:C	2.55	0.49
1:B:461:LEU:HD22	1:B:465:GLU:HB3	1.96	0.48
2:E:51:ILE:HG12	2:E:72:ARG:HD2	1.95	0.48
1:B:349:SER:O	1:B:352:ALA:O	2.31	0.48
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.49	0.47
2:C:83:MET:HE2	2:C:86:LEU:HD21	1.96	0.47
1:A:387:LEU:C	1:A:390:LEU:HG	2.39	0.47
1:A:349:SER:O	1:A:352:ALA:O	2.33	0.46
1:A:365:TYR:OH	1:A:390:LEU:HD11	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:SER:HA	1:B:524:VAL:HG22	1.97	0.46
1:B:372:ALA:HB1	1:B:373:PRO:HD2	1.98	0.46
1:B:334:ASN:O	1:B:334:ASN:OD1	2.34	0.46
2:E:20:LEU:HG	2:E:83:MET:HE2	1.97	0.46
1:B:472:ILE:H	1:B:472:ILE:HG12	1.54	0.45
1:A:387:LEU:O	1:A:390:LEU:HG	2.16	0.45
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.98	0.45
1:B:362:VAL:HA	1:B:525:CYS:O	2.17	0.45
2:C:64:VAL:HG13	2:C:68:PHE:HB2	1.98	0.45
2:E:22:CYS:HB3	2:E:79:LEU:HB3	1.97	0.44
2:C:168:LEU:O	2:C:177:PRO:HG3	2.17	0.44
2:E:60:TYR:HB2	2:E:65:LYS:HE3	2.00	0.43
2:E:144:GLY:O	2:E:191:ASN:HB3	2.18	0.43
2:C:102:THR:OG1	2:C:103:ALA:N	2.51	0.43
2:E:143:THR:HG23	2:E:192:THR:OG1	2.18	0.43
2:E:18:LEU:HB2	2:E:86:LEU:HD11	2.01	0.43
1:B:350:VAL:HG22	1:B:422:ASN:HB3	2.00	0.43
2:C:125:THR:OG1	2:C:143:THR:HB	2.18	0.43
1:A:360:ASN:N	1:A:523:THR:HG22	2.27	0.43
1:B:383:SER:HA	1:B:384:PRO:HD3	1.79	0.42
2:C:107:PHE:O	2:C:168:LEU:HD13	2.20	0.42
2:E:91:THR:HG23	2:E:117:THR:HA	2.00	0.42
2:C:107:PHE:O	2:C:168:LEU:CD1	2.68	0.42
2:E:142:CYS:O	2:E:192:THR:HA	2.19	0.42
1:B:379:CYS:SG	1:B:384:PRO:HG3	2.60	0.41
1:A:374:PHE:HD1	1:A:436:TRP:HB3	1.84	0.41
1:B:369:TYR:CG	1:B:370:ASN:N	2.82	0.41
1:A:439:ASN:HA	1:A:507:PRO:HG2	2.02	0.41
2:E:99:GLY:HA3	2:E:103:ALA:O	2.20	0.41
2:E:51:ILE:HD12	2:E:58:THR:HG22	2.03	0.41
1:A:421:TYR:O	1:A:461:LEU:HD11	2.21	0.41
1:A:517:LEU:HD23	1:A:517:LEU:HA	1.87	0.40
1:B:426:PRO:HG3	1:B:463:PRO:HB3	2.03	0.40
1:B:384:PRO:HA	1:B:387:LEU:HD12	2.03	0.40
2:C:86:LEU:HD23	2:C:86:LEU:HA	1.85	0.40
2:C:156:SER:O	2:C:211:CYS:N	2.50	0.40
2:E:12:VAL:HG11	2:E:18:LEU:HG	2.03	0.40
1:A:370:ASN:HD22	1:A:370:ASN:HA	1.69	0.40
2:E:52:SER:HB3	2:E:57:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

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	189/201 (94%)	183 (97%)	6 (3%)	0	100	100
1	B	172/201 (86%)	163 (95%)	8 (5%)	1 (1%)	21	38
2	C	223/232 (96%)	214 (96%)	9 (4%)	0	100	100
2	E	226/232 (97%)	217 (96%)	9 (4%)	0	100	100
All	All	810/866 (94%)	777 (96%)	32 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	ALA

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	163/170 (96%)	156 (96%)	7 (4%)	26	51
1	B	158/170 (93%)	147 (93%)	11 (7%)	14	29
2	C	182/184 (99%)	177 (97%)	5 (3%)	39	67
2	E	183/184 (100%)	171 (93%)	12 (7%)	15	32
All	All	686/708 (97%)	651 (95%)	35 (5%)	21	43

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	359	SER
1	A	367	VAL
1	A	370	ASN
1	A	371	PHE
1	A	394	ASN
1	A	472	ILE
1	A	523	THR
1	B	343	ASN
1	B	362	VAL
1	B	375	PHE
1	B	383	SER
1	B	385	THR
1	B	441	LEU
1	B	445	VAL
1	B	455	LEU
1	B	471	GLU
1	B	514	SER
1	B	524	VAL
2	C	20	LEU
2	C	30	ASN
2	C	64	VAL
2	C	147	SER
2	C	148	ASP
2	E	19	ARG
2	E	63	SER
2	E	64	VAL
2	E	65	LYS
2	E	119	SER
2	E	148	ASP
2	E	155	VAL
2	E	156	SER
2	E	194	SER
2	E	212	SER
2	E	216	THR
2	E	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	360	ASN
1	A	370	ASN
1	B	360	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	487	ASN
2	C	82	GLN
2	C	84	ASN
2	C	153	ASN
2	C	160	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	191/201 (95%)	1.15	43 (22%) 2 2	28, 49, 98, 105	0
1	B	180/201 (89%)	1.21	44 (24%) 2 1	31, 53, 91, 101	0
2	C	227/232 (97%)	0.10	3 (1%) 75 71	18, 33, 51, 70	9 (3%)
2	E	230/232 (99%)	0.23	8 (3%) 47 42	16, 32, 53, 63	8 (3%)
All	All	828/866 (95%)	0.62	98 (11%) 9 7	16, 39, 88, 105	17 (2%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	VAL	4.7
1	B	369	TYR	4.6
1	B	374	PHE	4.6
1	A	390	LEU	4.6
1	A	392	PHE	4.5
1	B	371	PHE	4.5
1	B	389	ASP	4.5
1	A	369	TYR	4.4
1	B	456	PHE	4.2
1	B	479	PRO	4.2
1	A	480	CYS	4.1
1	B	526	GLY	4.0
1	A	391	CYS	3.9
1	B	368	LEU	3.8
1	A	520	ALA	3.8
1	A	517	LEU	3.7
1	B	377	PHE	3.6
1	B	385	THR	3.5
1	B	370	ASN	3.5
1	A	486	VAL	3.5
1	B	515	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	372	ALA	3.4
1	A	478	LYS	3.4
1	B	487	ASN	3.4
1	A	518	LEU	3.2
1	B	372	ALA	3.1
1	B	390	LEU	3.1
1	B	475	ALA	3.1
2	E	229	LEU	3.0
1	A	371	PHE	3.0
1	A	368	LEU	3.0
1	A	387	LEU	3.0
1	A	365	TYR	2.9
1	B	396	TYR	2.9
1	B	441	LEU	2.9
1	A	526	GLY	2.9
1	A	382	VAL	2.9
1	A	479	PRO	2.9
2	C	98	ASN	2.9
1	A	525	CYS	2.9
1	B	525	CYS	2.9
1	B	383	SER	2.9
2	E	30	ASN	2.9
1	B	514	SER	2.8
2	C	120	SER	2.8
1	B	367	VAL	2.8
1	A	488	CYS	2.8
1	A	375	PHE	2.8
1	B	474	GLN	2.8
1	A	514	SER	2.8
1	A	521	PRO	2.8
1	A	340	GLU	2.8
1	A	339	ASP	2.7
1	B	523	THR	2.7
2	E	99	GLY	2.7
1	B	373	PRO	2.7
1	B	375	PHE	2.6
1	A	484	ALA	2.6
1	B	430	THR	2.6
1	A	367	VAL	2.6
1	B	365	TYR	2.6
1	A	483	VAL	2.6
1	A	393	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	2.6
1	A	377	PHE	2.5
1	B	388	ASN	2.5
1	B	477	ASN	2.5
1	A	383	SER	2.5
1	B	391	CYS	2.5
2	E	230	ALA	2.5
1	A	519	HIS	2.5
2	E	212	SER	2.5
1	A	373	PRO	2.5
1	A	489	TYR	2.5
2	E	231	ALA	2.5
1	B	393	THR	2.4
1	B	334	ASN	2.4
1	A	366	SER	2.3
1	B	524	VAL	2.3
1	A	481	ASN	2.3
1	B	335	LEU	2.2
1	B	366	SER	2.2
1	A	352	ALA	2.2
1	A	476	GLY	2.2
1	B	480	CYS	2.2
1	B	488	CYS	2.2
2	E	68	PHE	2.2
2	C	214	ALA	2.1
1	B	458	LYS	2.1
1	A	475	ALA	2.1
1	B	352	ALA	2.1
1	B	394	ASN	2.1
1	A	389	ASP	2.1
2	E	18	LEU	2.1
1	A	472	ILE	2.1
1	B	478	LYS	2.1
1	A	374	PHE	2.0
1	A	477	ASN	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.