



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:41 AM UTC

PDB ID : 8IEE / pdb_00008iee
Title : Crystal structure of nanobody VHH-31 with MERS-CoV RBD
Authors : Wang, X.; Tian, L.
Deposited on : 2023-02-15
Resolution : 3.21 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

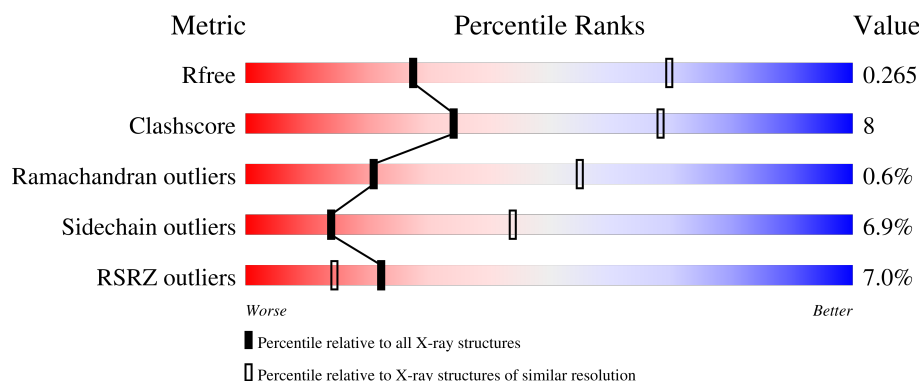
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	229	5% 67% 21% 10%
1	B	229	3% 66% 23% 10%
2	C	131	13% 69% 26% 5%
2	D	131	8% 73% 26% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5194 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	B	207	Total	C	N	O	S	0	0	0
			1600	1020	255	314	11			
1	A	207	Total	C	N	O	S	0	0	0
			1600	1020	255	314	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	590	HIS	-	expression tag	UNP R9UQ53
B	591	HIS	-	expression tag	UNP R9UQ53
B	592	HIS	-	expression tag	UNP R9UQ53
B	593	HIS	-	expression tag	UNP R9UQ53
B	594	HIS	-	expression tag	UNP R9UQ53
B	595	HIS	-	expression tag	UNP R9UQ53
A	590	HIS	-	expression tag	UNP R9UQ53
A	591	HIS	-	expression tag	UNP R9UQ53
A	592	HIS	-	expression tag	UNP R9UQ53
A	593	HIS	-	expression tag	UNP R9UQ53
A	594	HIS	-	expression tag	UNP R9UQ53
A	595	HIS	-	expression tag	UNP R9UQ53

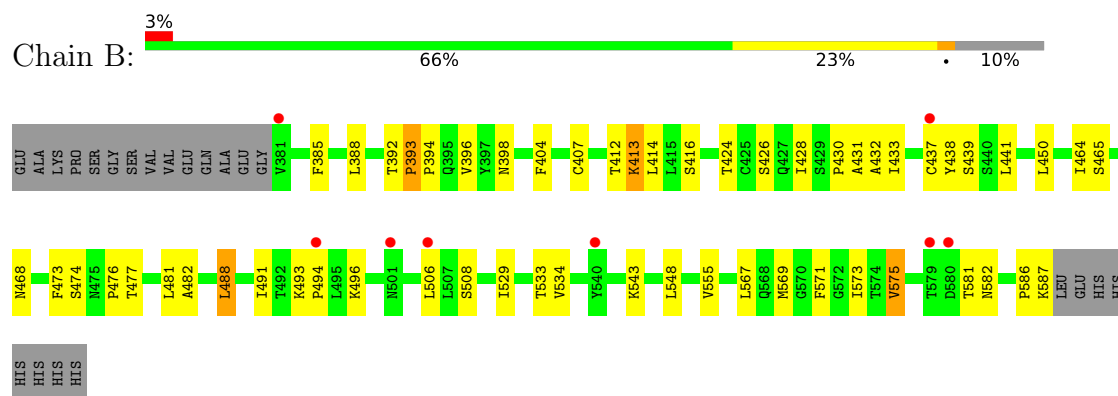
- Molecule 2 is a protein called VHH-31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	131	Total	C	N	O	S	0	0	0
			997	612	176	202	7			
2	C	131	Total	C	N	O	S	0	0	0
			997	612	176	202	7			

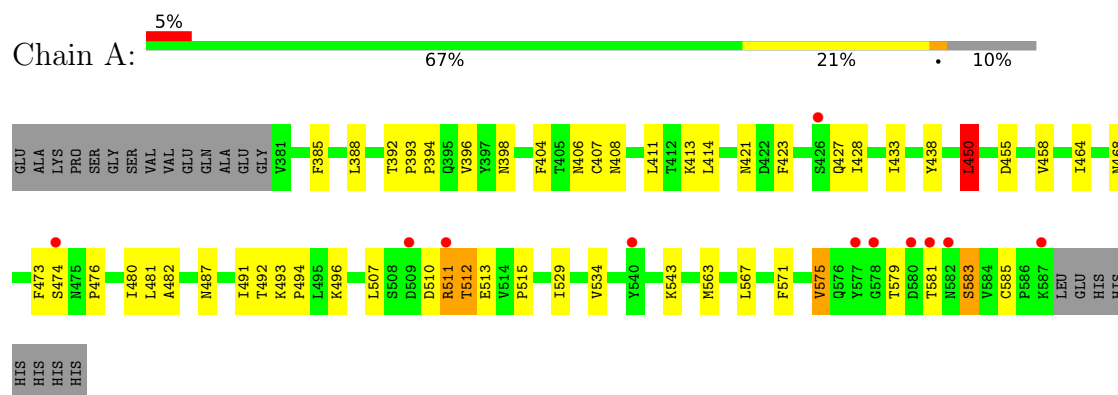
3 Residue-property plots [i](#)

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.

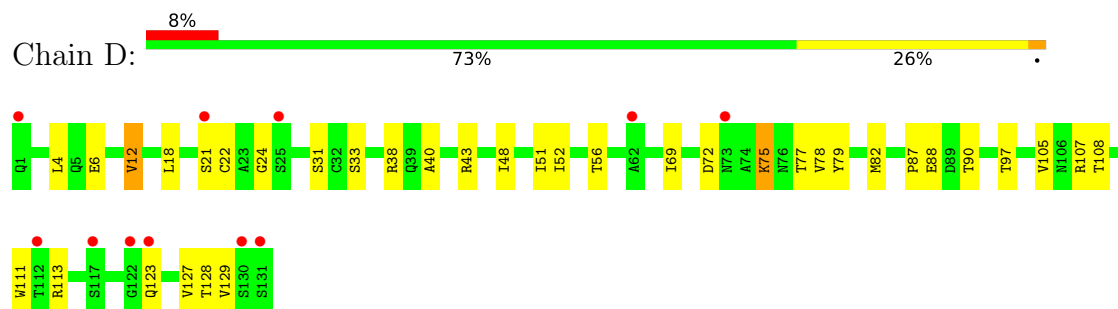
• Molecule 1: Spike protein S1



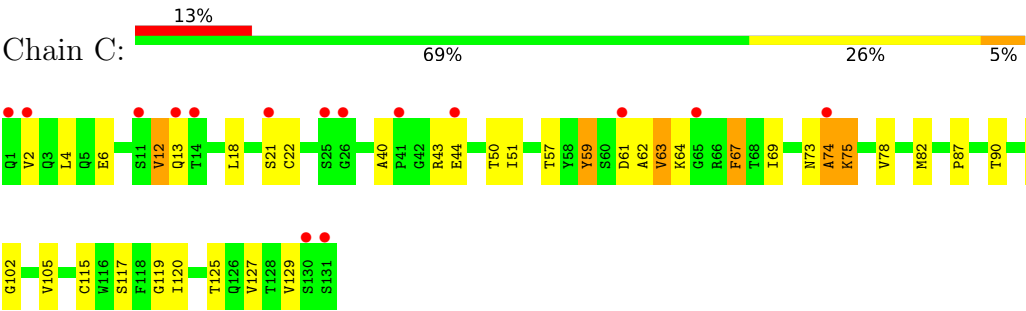
• Molecule 1: Spike protein S1



• Molecule 2: VHH-31



• Molecule 2: VHH-31



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.02Å 158.02Å 132.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.81 – 3.21 26.81 – 3.21	Depositor EDS
% Data completeness (in resolution range)	80.2 (26.81-3.21) 80.2 (26.81-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.24Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.243 , 0.252 0.249 , 0.265	Depositor DCC
R_{free} test set	1373 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5194	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	0.94	1/1639 (0.1%)	1.38	11/2238 (0.5%)
1	B	0.94	1/1639 (0.1%)	1.35	6/2238 (0.3%)
2	C	0.90	1/1016 (0.1%)	1.37	7/1377 (0.5%)
2	D	0.87	0/1016	1.40	6/1377 (0.4%)
All	All	0.92	3/5310 (0.1%)	1.37	30/7230 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	100	SER	CA-CB	-6.99	1.47	1.53
1	B	393	PRO	C-O	-5.24	1.20	1.24
1	A	393	PRO	C-O	-5.20	1.20	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	430	PRO	N-CA-C	-9.04	97.12	111.03
1	A	511	ARG	N-CA-C	-8.22	103.15	113.01
2	C	73	ASN	CB-CA-C	7.38	122.56	110.90
1	B	430	PRO	CA-C-O	-7.33	113.39	121.23
2	C	63	VAL	N-CA-C	-7.12	105.60	112.29
1	A	581	THR	CB-CA-C	6.91	121.88	111.80
1	A	510	ASP	CB-CA-C	6.79	122.61	111.26
2	D	31	SER	N-CA-C	-6.60	104.54	112.59
2	C	62	ALA	N-CA-C	-6.51	105.63	113.97
1	A	510	ASP	N-CA-C	-6.21	105.65	113.23
2	C	75	LYS	N-CA-C	-6.19	103.66	110.91
2	C	74	ALA	N-CA-C	-6.06	101.51	110.48
1	A	473	PHE	CA-C-O	-6.05	115.21	121.87
1	B	450	LEU	N-CA-C	-6.02	105.79	113.01
1	A	513	GLU	N-CA-C	6.01	119.06	110.10
1	B	385	PHE	N-CA-C	-5.86	105.71	112.92
1	B	430	PRO	CB-CA-C	-5.68	104.49	111.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	75	LYS	N-CA-C	-5.58	99.64	108.73
2	D	107	ARG	N-CA-C	-5.39	105.41	111.28
2	C	74	ALA	CA-C-O	-5.37	115.29	121.47
1	A	450	LEU	N-CA-C	-5.35	106.59	113.01
1	A	385	PHE	N-CA-C	-5.31	106.66	112.72
1	A	458	VAL	N-CA-C	-5.29	106.71	112.80
1	A	512	THR	CB-CA-C	5.15	120.67	110.42
2	D	56	THR	CB-CA-C	5.13	117.90	109.90
2	C	59	TYR	CB-CA-C	5.11	118.72	109.37
2	D	108	THR	CA-C-O	-5.10	116.00	121.56
1	B	432	ALA	N-CA-C	-5.03	105.88	111.36
1	A	579	THR	O-C-N	5.02	125.23	120.71
2	D	108	THR	N-CA-C	-5.00	103.45	110.50

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	1600	0	1563	19	0
1	B	1600	0	1563	21	0
2	C	997	0	942	19	4
2	D	997	0	942	20	4
All	All	5194	0	5010	78	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:CYS:HB3	2:C:78:VAL:HG12	1.73	0.70
1:B:404:PHE:HB3	1:B:407:CYS:SG	2.35	0.67
1:A:388:LEU:HD23	1:A:414:LEU:HD11	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:VAL:HG13	2:C:129:VAL:HG22	1.81	0.63
2:D:4:LEU:HD11	2:D:97:THR:HG22	1.81	0.62
1:B:437:CYS:SG	1:B:582:ASN:HA	2.41	0.61
1:B:428:ILE:HB	1:B:476:PRO:HB3	1.87	0.57
1:A:428:ILE:HB	1:A:476:PRO:HB3	1.88	0.55
2:C:63:VAL:HB	2:C:67:PHE:HB2	1.88	0.55
1:B:494:PRO:HD2	1:B:567:LEU:HD13	1.89	0.55
2:D:22:CYS:HB3	2:D:78:VAL:HG12	1.90	0.54
1:B:388:LEU:HD23	1:B:414:LEU:HD11	1.90	0.54
1:A:433:ILE:HA	1:A:438:TYR:HE2	1.73	0.54
2:C:51:ILE:HG13	2:C:57:THR:HG22	1.88	0.54
1:B:433:ILE:HA	1:B:438:TYR:HE2	1.73	0.53
2:D:90:THR:HG23	2:D:128:THR:HA	1.90	0.53
1:A:406:ASN:H	1:A:583:SER:HB2	1.75	0.52
1:A:476:PRO:HB2	1:A:575:VAL:HG22	1.91	0.52
1:A:493:LYS:HG2	1:A:567:LEU:HB2	1.92	0.52
2:D:82:MET:HE1	2:D:127:VAL:HG11	1.92	0.51
2:C:59:TYR:HE1	2:C:69:ILE:HG13	1.74	0.51
2:D:4:LEU:HB3	2:D:22:CYS:SG	2.51	0.51
1:B:496:LYS:HD2	1:B:534:VAL:O	2.11	0.51
1:A:494:PRO:HD2	1:A:567:LEU:HD13	1.93	0.50
2:C:61:ASP:HA	2:C:64:LYS:HG3	1.94	0.50
1:A:404:PHE:HB3	1:A:407:CYS:SG	2.52	0.49
1:A:482:ALA:HB3	1:A:571:PHE:HE1	1.77	0.49
2:C:40:ALA:HB3	2:C:43:ARG:HB3	1.94	0.49
1:B:488:LEU:HD22	1:B:491:ILE:HG13	1.94	0.49
1:B:413:LYS:HG3	1:B:414:LEU:N	2.27	0.49
2:D:123:GLN:H	2:D:123:GLN:CD	2.19	0.49
1:B:394:PRO:HB2	1:B:398:ASN:O	2.13	0.48
2:D:72:ASP:HB3	2:D:75:LYS:O	2.13	0.48
1:B:464:ILE:HA	1:B:468:ASN:HB2	1.96	0.48
2:D:87:PRO:HA	2:D:129:VAL:HB	1.95	0.48
2:D:40:ALA:HB3	2:D:43:ARG:HB2	1.95	0.47
1:A:464:ILE:HA	1:A:468:ASN:HB2	1.96	0.47
1:A:529:ILE:HG21	1:A:543:LYS:HB2	1.96	0.46
2:D:111:TRP:CZ2	2:D:113:ARG:HG3	2.51	0.46
2:D:90:THR:HA	2:D:127:VAL:O	2.16	0.46
1:A:421:ASN:CB	1:A:450:LEU:HD21	2.46	0.46
2:C:44:GLU:H	2:C:44:GLU:CD	2.24	0.46
2:C:6:GLU:HA	2:C:21:SER:O	2.16	0.45
1:A:496:LYS:HD2	1:A:534:VAL:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:ILE:HG21	1:B:543:LYS:HB2	1.99	0.45
1:A:423:PHE:CD1	1:A:480:ILE:HG12	2.51	0.45
2:D:12:VAL:HG23	2:D:129:VAL:HG22	1.98	0.45
2:D:38:ARG:HD3	2:D:48:ILE:HD11	1.99	0.45
2:C:87:PRO:O	2:C:90:THR:HG22	2.17	0.45
1:B:412:THR:O	1:B:416:SER:HB3	2.17	0.45
2:D:33:SER:O	2:D:97:THR:HA	2.17	0.44
2:D:18:LEU:HD23	2:D:18:LEU:HA	1.89	0.44
1:B:493:LYS:HG2	1:B:567:LEU:HB2	1.98	0.44
1:B:496:LYS:HG2	1:B:533:THR:HG22	1.99	0.44
2:D:88:GLU:H	2:D:88:GLU:HG3	1.54	0.44
2:C:22:CYS:HB3	2:C:78:VAL:CG1	2.46	0.44
2:D:69:ILE:HA	2:D:79:TYR:O	2.19	0.43
1:A:408:ASN:HA	1:A:585:CYS:O	2.17	0.43
2:D:22:CYS:O	2:D:77:THR:HA	2.18	0.43
2:C:99:TRP:CZ2	2:C:119:GLY:HA3	2.54	0.43
2:C:82:MET:HE3	2:C:82:MET:HB2	1.93	0.43
1:B:392:THR:HA	1:B:393:PRO:HD3	1.89	0.43
1:A:394:PRO:HB2	1:A:398:ASN:O	2.19	0.43
1:A:515:PRO:HD2	2:C:50:THR:OG1	2.18	0.43
2:C:12:VAL:O	2:C:129:VAL:HA	2.20	0.42
1:B:473:PHE:HA	1:B:477:THR:HG21	2.01	0.42
2:C:102:GLY:O	2:C:115:CYS:HB2	2.19	0.42
2:D:6:GLU:HA	2:D:21:SER:O	2.20	0.42
2:C:4:LEU:HD11	2:C:97:THR:HG22	2.02	0.42
1:B:482:ALA:HB3	1:B:571:PHE:HE1	1.86	0.41
1:B:569:MET:HB3	1:B:569:MET:HE2	1.68	0.41
2:C:90:THR:HA	2:C:127:VAL:O	2.21	0.41
1:B:441:LEU:HD12	1:B:575:VAL:HG12	2.03	0.41
1:A:507:LEU:HD12	1:A:511:ARG:HB2	2.03	0.41
1:A:563:MET:HB2	1:A:563:MET:HE2	1.72	0.41
2:D:4:LEU:HD23	2:D:24:GLY:HA2	2.02	0.41
2:C:74:ALA:O	2:C:75:LYS:HB2	2.22	0.40
1:B:587:LYS:HE3	1:B:587:LYS:HB3	1.86	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:ARG:NE	2:C:13:GLN:NE2[2_565]	1.23	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:ARG:CD	2:C:13:GLN:NE2[2_565]	1.53	0.67
2:D:113:ARG:CZ	2:C:13:GLN:NE2[2_565]	1.70	0.50
2:D:113:ARG:NH1	2:C:13:GLN:NE2[2_565]	2.17	0.03

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	205/229 (90%)	196 (96%)	7 (3%)	2 (1%)	12	44
1	B	205/229 (90%)	195 (95%)	8 (4%)	2 (1%)	12	44
2	C	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
2	D	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
All	All	668/720 (93%)	638 (96%)	26 (4%)	4 (1%)	21	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	431	ALA
1	B	586	PRO
1	A	474	SER
1	A	512	THR

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	189/207 (91%)	176 (93%)	13 (7%)	14	44
1	B	189/207 (91%)	173 (92%)	16 (8%)	10	35
2	C	108/108 (100%)	100 (93%)	8 (7%)	13	41
2	D	108/108 (100%)	104 (96%)	4 (4%)	30	60
All	All	594/630 (94%)	553 (93%)	41 (7%)	14	44

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	396	VAL
1	B	413	LYS
1	B	424	THR
1	B	426	SER
1	B	439	SER
1	B	465	SER
1	B	474	SER
1	B	481	LEU
1	B	488	LEU
1	B	506	LEU
1	B	508	SER
1	B	548	LEU
1	B	555	VAL
1	B	573	ILE
1	B	575	VAL
1	B	581	THR
2	D	12	VAL
2	D	51	ILE
2	D	52	ILE
2	D	105	VAL
1	A	392	THR
1	A	396	VAL
1	A	411	LEU
1	A	413	LYS
1	A	427	GLN
1	A	450	LEU
1	A	455	ASP
1	A	481	LEU
1	A	487	ASN
1	A	491	ILE
1	A	492	THR
1	A	575	VAL
1	A	583	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	2	VAL
2	C	12	VAL
2	C	18	LEU
2	C	67	PHE
2	C	105	VAL
2	C	117	SER
2	C	120	ILE
2	C	125	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	421	ASN
1	B	566	GLN
1	A	421	ASN
1	A	522	GLN
2	C	73	ASN

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 ⓘ

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	207/229 (90%)	0.56	11 (5%) 32 20	30, 44, 62, 82	0
1	B	207/229 (90%)	0.47	8 (3%) 43 27	27, 43, 63, 84	0
2	C	131/131 (100%)	0.84	17 (12%) 7 6	31, 54, 78, 112	0
2	D	131/131 (100%)	0.81	11 (8%) 17 11	30, 47, 73, 103	0
All	All	676/720 (93%)	0.64	47 (6%) 22 14	27, 46, 70, 112	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	581	THR	4.9
1	A	426	SER	4.9
2	C	1	GLN	4.3
1	A	587	LYS	3.7
2	D	131	SER	3.6
1	A	511	ARG	3.6
2	D	1	GLN	3.5
2	D	117	SER	3.3
1	A	509	ASP	3.2
2	C	98	GLY	3.2
1	B	580	ASP	3.1
2	D	62	ALA	3.1
1	A	580	ASP	3.1
2	C	101	GLN	3.0
2	C	131	SER	3.0
2	D	25	SER	2.9
2	D	122	GLY	2.9
1	B	437	CYS	2.9
2	C	130	SER	2.9
1	B	579	THR	2.9
2	C	61	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	44	GLU	2.7
2	D	21	SER	2.6
2	C	2	VAL	2.5
2	C	11	SER	2.5
2	C	25	SER	2.5
1	A	577	TYR	2.5
2	C	26	GLY	2.4
2	D	130	SER	2.4
2	C	14	THR	2.3
1	A	582	ASN	2.3
2	C	65	GLY	2.3
2	D	123	GLN	2.3
1	A	474	SER	2.3
1	B	381	VAL	2.3
1	A	578	GLY	2.2
2	C	13	GLN	2.1
1	B	494	PRO	2.1
1	B	506	LEU	2.1
1	B	501	ASN	2.1
1	A	540	TYR	2.1
2	D	112	THR	2.1
2	C	74	ALA	2.1
2	C	41	PRO	2.1
2	C	21	SER	2.0
2	D	73	ASN	2.0
1	B	540	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.