



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:44 PM UTC

PDB ID : 5CFD / pdb\_00005cfd  
Title : Crystal Structure of DTT treated Human Coronavirus SAFV-3  
Authors : Mullapudi, E.; Plevka, P.  
Deposited on : 2015-07-08  
Resolution : 2.50 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

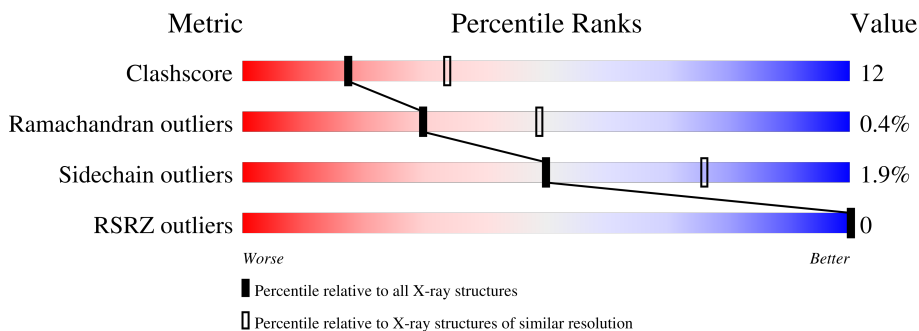
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
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  $\geq 3$ , 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	252	74% (green), 25% (yellow), 1% (orange), 0% (red)
2	B	232	75% (green), 22% (yellow), 1% (orange), 0% (red)
3	C	258	69% (green), 28% (yellow), 1% (orange), 0% (red)
4	D	24	63% (green), 21% (yellow), 12% (orange), 4% (red)

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6350 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	1996	1273	332	384	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	PHE	VAL	conflict	UNP COMHL9

- Molecule 2 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	232	1804	1166	285	343	10	0	0	0

- Molecule 3 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	258	2023	1274	364	378	7	0	0	0

- Molecule 4 is a protein called VP4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	24	189	115	32	42	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		

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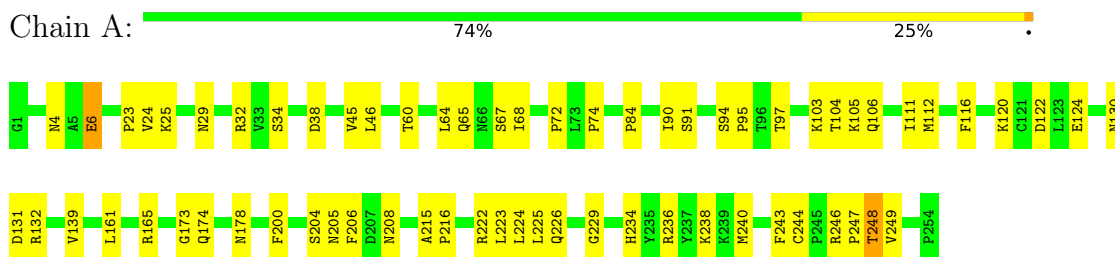
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	B	99	Total O 99 99	0	0
5	C	107	Total O 107 107	0	0
5	D	8	Total O 8 8	0	0

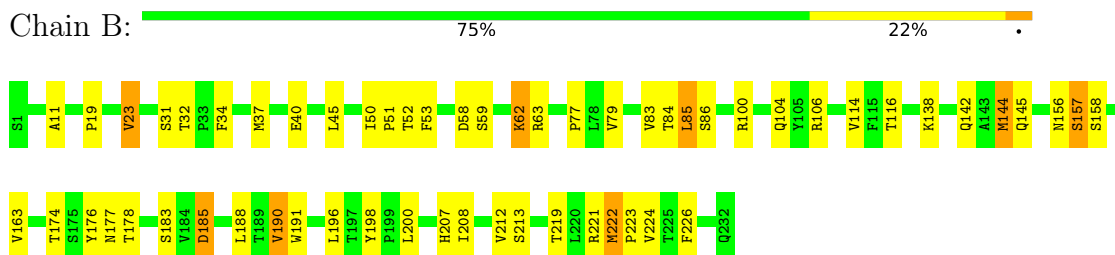
### 3 Residue-property plots

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.

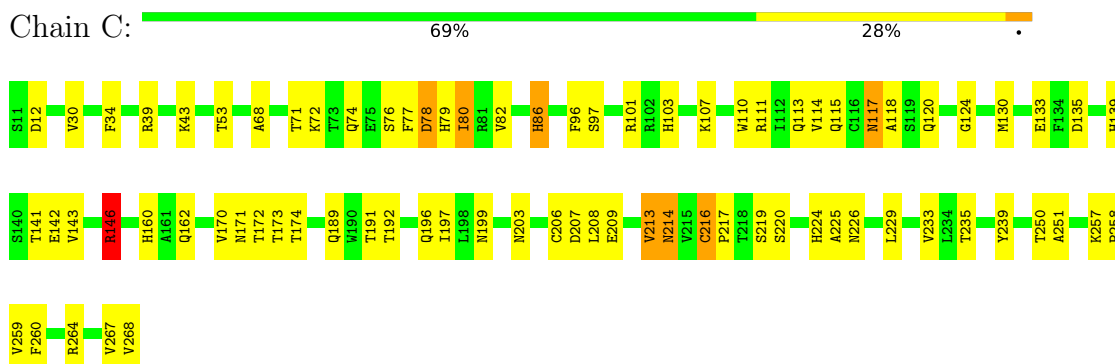
- Molecule 1: VP1



- Molecule 2: VP3



- Molecule 3: VP2



- Molecule 4: VP4





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	299.95Å 299.95Å 723.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.00 – 2.50 70.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	67.4 (70.00-2.50) 67.5 (70.00-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.51Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , (Not available) 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtrriage
Anisotropy	0.097	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 98.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.58$ , $\langle L^2 \rangle = 0.43$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.44	EDS
Total number of atoms	6350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.03	19/2055 (0.9%)	1.10	20/2808 (0.7%)
2	B	1.43	27/1860 (1.5%)	1.13	19/2553 (0.7%)
3	C	1.66	33/2078 (1.6%)	1.28	26/2843 (0.9%)
4	D	2.95	16/191 (8.4%)	1.66	8/259 (3.1%)
All	All	1.47	95/6184 (1.5%)	1.19	73/8463 (0.9%)

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
3	C	0	1

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	259	VAL	C-O	-25.61	0.96	1.24
2	B	212	VAL	C-O	-23.11	0.98	1.23
3	C	203	ASN	C-O	-21.19	0.98	1.23
3	C	214	ASN	C-O	-21.14	1.00	1.23
2	B	23	VAL	C-O	-20.81	0.98	1.24
3	C	111	ARG	C-O	-20.18	1.01	1.24
2	B	63	ARG	C-O	-20.11	1.00	1.24
4	D	28	GLN	C-O	-20.10	0.98	1.24
3	C	199	ASN	C-O	-18.92	1.00	1.24
1	A	240	MET	C-O	-18.80	1.01	1.23
3	C	118	ALA	C-O	-18.08	1.01	1.24
1	A	132	ARG	C-O	-17.52	1.00	1.24
3	C	226	ASN	C-O	-16.33	1.03	1.24
3	C	226	ASN	CG-ND2	-14.67	1.02	1.33
2	B	23	VAL	CA-C	-14.18	1.38	1.52
2	B	200	LEU	C-O	-13.38	1.05	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	203	ASN	CG-ND2	-13.10	1.05	1.33
4	D	20	ILE	C-O	-12.75	1.06	1.24
3	C	203	ASN	CG-OD1	-12.35	1.00	1.23
3	C	162	GLN	C-N	-12.20	1.21	1.33
1	A	240	MET	SD-CE	-12.02	1.49	1.79
2	B	145	GLN	C-O	-11.92	1.08	1.24
2	B	145	GLN	N-CA	-11.29	1.31	1.46
2	B	63	ARG	CZ-NH2	-11.28	1.18	1.33
3	C	111	ARG	CZ-NH2	-11.07	1.19	1.33
2	B	144	MET	C-O	-10.98	1.09	1.24
1	A	205	ASN	CG-ND2	-10.90	1.10	1.33
2	B	145	GLN	CD-OE1	-10.78	1.03	1.23
3	C	146	ARG	CZ-NH2	-10.77	1.19	1.33
2	B	63	ARG	CZ-NH1	-10.47	1.18	1.32
2	B	145	GLN	CD-NE2	-10.47	1.11	1.33
3	C	111	ARG	CZ-NH1	-9.81	1.19	1.32
1	A	132	ARG	C-N	-9.78	1.20	1.33
4	D	20	ILE	N-CA	-9.71	1.33	1.46
4	D	17	GLU	C-N	-9.69	1.19	1.33
4	D	28	GLN	CA-C	-9.64	1.38	1.52
2	B	144	MET	SD-CE	-9.59	1.55	1.79
3	C	214	ASN	CG-OD1	-9.59	1.05	1.23
2	B	63	ARG	CD-NE	-9.41	1.33	1.46
4	D	17	GLU	C-O	-9.32	1.12	1.24
3	C	226	ASN	CG-OD1	-9.01	1.06	1.23
3	C	111	ARG	CA-C	-8.87	1.42	1.52
4	D	16	ASN	CA-C	-8.80	1.41	1.52
1	A	240	MET	CG-SD	-8.77	1.58	1.80
3	C	146	ARG	C-O	-8.76	1.12	1.23
3	C	213	VAL	C-N	-8.71	1.22	1.33
4	D	16	ASN	C-O	-8.62	1.13	1.24
1	A	205	ASN	CG-OD1	-8.55	1.07	1.23
3	C	214	ASN	CG-ND2	-8.53	1.15	1.33
3	C	111	ARG	CD-NE	-8.43	1.34	1.46
3	C	117	ASN	C-N	-8.30	1.22	1.33
3	C	199	ASN	CG-OD1	-8.25	1.07	1.23
3	C	199	ASN	CG-ND2	-8.07	1.16	1.33
1	A	205	ASN	C-O	-7.84	1.13	1.23
1	A	174	GLN	N-CA	-7.81	1.35	1.46
3	C	162	GLN	C-O	-7.73	1.11	1.24
4	D	28	GLN	C-N	-7.70	1.22	1.33
2	B	63	ARG	C-N	-7.41	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ARG	CZ-NH2	-7.35	1.23	1.33
2	B	144	MET	CG-SD	-7.24	1.62	1.80
2	B	144	MET	C-N	-7.04	1.22	1.33
3	C	259	VAL	C-N	-6.87	1.23	1.33
4	D	17	GLU	N-CA	-6.86	1.38	1.46
2	B	23	VAL	C-N	-6.61	1.28	1.33
4	D	15	GLY	C-N	-6.59	1.24	1.33
1	A	132	ARG	CD-NE	-6.52	1.37	1.46
1	A	132	ARG	N-CA	-6.46	1.38	1.46
2	B	212	VAL	N-CA	-6.36	1.39	1.46
3	C	225	ALA	C-N	-6.26	1.25	1.34
4	D	17	GLU	CD-OE1	-6.26	1.13	1.25
4	D	16	ASN	CG-OD1	-6.24	1.11	1.23
1	A	132	ARG	CA-CB	-6.16	1.44	1.53
4	D	20	ILE	CA-C	-6.15	1.43	1.52
3	C	162	GLN	N-CA	-6.11	1.37	1.46
4	D	19	VAL	C-N	-5.70	1.26	1.33
3	C	111	ARG	CA-CB	-5.69	1.44	1.53
2	B	212	VAL	CA-C	-5.65	1.46	1.52
2	B	62	LYS	C-N	-5.60	1.25	1.33
1	A	240	MET	N-CA	-5.57	1.39	1.46
2	B	200	LEU	N-CA	-5.55	1.38	1.45
1	A	240	MET	C-N	-5.52	1.25	1.33
2	B	212	VAL	CA-CB	-5.46	1.45	1.55
2	B	200	LEU	CG-CD1	-5.41	1.34	1.52
3	C	214	ASN	C-N	-5.36	1.27	1.34
1	A	174	GLN	CG-CD	-5.32	1.38	1.52
2	B	145	GLN	C-N	-5.31	1.26	1.33
4	D	15	GLY	C-O	-5.30	1.12	1.23
1	A	131	ASP	C-N	-5.29	1.26	1.33
2	B	23	VAL	CA-CB	5.25	1.60	1.54
1	A	205	ASN	CA-C	5.16	1.59	1.52
3	C	199	ASN	CA-CB	-5.15	1.46	1.53
1	A	240	MET	CA-C	-5.13	1.46	1.52
3	C	111	ARG	CG-CD	-5.13	1.37	1.52
2	B	145	GLN	CG-CD	-5.03	1.39	1.52
3	C	111	ARG	N-CA	-5.02	1.40	1.46

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	259	VAL	CA-C-N	-14.87	100.64	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	259	VAL	C-N-CA	-14.87	100.64	122.94
3	C	259	VAL	O-C-N	11.31	136.33	123.10
1	A	132	ARG	N-CA-C	11.26	125.55	112.93
1	A	132	ARG	CG-CD-NE	-10.55	88.80	112.00
3	C	258	PRO	CA-C-N	10.55	136.83	123.12
3	C	258	PRO	C-N-CA	10.55	136.83	123.12
3	C	259	VAL	N-CA-C	10.37	122.84	107.80
4	D	17	GLU	CA-C-O	9.35	131.39	119.98
3	C	203	ASN	N-CA-C	9.20	124.61	109.24
1	A	174	GLN	CA-C-O	-8.84	107.97	119.10
3	C	12	ASP	N-CA-C	-8.75	102.60	113.18
1	A	173	GLY	O-C-N	8.60	133.88	122.70
4	D	17	GLU	CB-CA-C	8.17	121.78	110.34
2	B	53	PHE	N-CA-C	8.11	122.28	110.28
3	C	78	ASP	N-CA-C	-7.83	98.68	110.28
2	B	200	LEU	CA-C-O	-7.68	113.42	121.87
1	A	229	GLY	N-CA-C	7.49	119.79	111.85
3	C	219	SER	N-CA-C	7.47	122.00	109.76
3	C	226	ASN	N-CA-C	7.39	120.40	111.82
2	B	212	VAL	CA-C-O	-7.02	114.68	121.63
3	C	146	ARG	NE-CZ-NH1	6.92	128.42	121.50
3	C	220	SER	N-CA-C	-6.91	99.25	109.62
3	C	214	ASN	N-CA-C	6.62	118.21	108.14
2	B	63	ARG	CB-CG-CD	6.59	126.46	111.30
4	D	20	ILE	CA-C-O	-6.58	113.14	120.25
2	B	196	LEU	N-CA-C	-6.49	100.23	109.96
2	B	157	SER	N-CA-C	6.45	120.36	112.23
2	B	62	LYS	O-C-N	-6.43	115.67	123.19
2	B	198	TYR	N-CA-C	6.42	113.78	108.07
3	C	259	VAL	N-CA-CB	-6.36	103.45	111.46
1	A	178	ASN	N-CA-C	6.35	120.28	111.90
2	B	222	MET	N-CA-C	6.28	123.68	109.81
4	D	28	GLN	N-CA-C	6.27	120.49	112.34
2	B	59	SER	N-CA-C	-6.14	105.27	112.89
3	C	259	VAL	CB-CA-C	6.13	119.91	110.96
1	A	240	MET	N-CA-C	6.10	119.11	109.96
2	B	163	VAL	N-CA-C	-6.00	102.10	107.56
2	B	63	ARG	N-CA-C	5.96	118.35	109.59
1	A	23	PRO	N-CA-C	-5.94	101.93	111.38
1	A	206	PHE	N-CA-C	5.92	119.76	112.54
1	A	205	ASN	CA-C-O	-5.90	114.71	121.68
1	A	122	ASP	N-CA-C	-5.87	101.32	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	212	VAL	N-CA-CB	-5.85	101.54	112.36
1	A	165	ARG	N-CA-C	-5.78	106.27	113.38
1	A	97	THR	N-CA-C	5.71	118.25	111.33
3	C	96	PHE	N-CA-C	-5.69	105.00	111.14
1	A	174	GLN	CA-C-N	5.67	132.52	121.41
1	A	174	GLN	C-N-CA	5.67	132.52	121.41
2	B	62	LYS	CA-C-N	5.65	129.38	121.24
2	B	62	LYS	C-N-CA	5.65	129.38	121.24
2	B	37	MET	N-CA-C	5.65	118.03	110.35
3	C	162	GLN	N-CA-C	5.61	119.66	113.21
4	D	17	GLU	N-CA-C	-5.61	98.67	107.93
2	B	185	ASP	N-CA-C	5.59	119.28	111.56
1	A	130	ASN	N-CA-C	5.52	119.76	113.19
3	C	86	HIS	N-CA-C	5.52	118.01	111.33
3	C	53	THR	N-CA-C	-5.40	100.44	109.24
3	C	79	HIS	N-CA-C	5.32	116.88	108.96
3	C	30	VAL	N-CA-C	-5.30	106.26	111.88
3	C	172	THR	N-CA-C	5.28	118.51	111.75
2	B	85	LEU	N-CA-C	-5.26	106.11	113.37
4	D	17	GLU	CB-CG-CD	5.25	121.53	112.60
4	D	20	ILE	N-CA-C	5.24	118.47	111.44
2	B	177	ASN	N-CA-C	-5.21	104.55	112.04
1	A	25	LYS	N-CA-C	5.17	117.93	110.28
1	A	205	ASN	CA-C-N	5.14	129.31	120.72
1	A	205	ASN	C-N-CA	5.14	129.31	120.72
3	C	216	CYS	CA-C-N	5.09	126.20	119.84
3	C	216	CYS	C-N-CA	5.09	126.20	119.84
1	A	240	MET	CB-CG-SD	5.08	127.95	112.70
3	C	226	ASN	CA-C-O	-5.05	114.16	119.97
4	D	28	GLN	CA-CB-CG	5.04	124.18	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	117	ASN	Mainchain

## 5.2 Too-close contacts [i](#)

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	1996	0	1938	50	0
2	B	1804	0	1761	55	0
3	C	2023	0	1961	63	0
4	D	189	0	167	8	0
5	A	124	0	0	3	0
5	B	99	0	0	2	0
5	C	107	0	0	2	0
5	D	8	0	0	0	0
All	All	6350	0	5827	148	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 12.

All (148) 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:46:LEU:HD13	1:A:68:ILE:HG23	1.46	0.97
2:B:138:LYS:H	2:B:142:GLN:NE2	1.68	0.90
1:A:104:THR:HG23	1:A:106:GLN:OE1	1.74	0.87
1:A:238:LYS:NZ	4:D:17:GLU:OE2	2.09	0.81
2:B:104:GLN:HE22	2:B:221:ARG:HH21	1.28	0.81
1:A:248:THR:H	3:C:189:GLN:HE22	1.30	0.78
3:C:97:SER:O	3:C:101:ARG:HG3	1.84	0.77
3:C:71:THR:H	3:C:74:GLN:NE2	1.84	0.76
3:C:113:GLN:HE21	3:C:115:GLN:HE21	1.34	0.73
2:B:116:THR:HG21	3:C:235:THR:HG21	1.68	0.73
1:A:161:LEU:H	1:A:226:GLN:HE22	1.36	0.73
2:B:138:LYS:H	2:B:142:GLN:HE21	1.32	0.73
1:A:124:GLU:HB3	1:A:236:ARG:HB3	1.71	0.71
1:A:248:THR:H	3:C:189:GLN:NE2	1.87	0.71
3:C:34:PHE:CE1	3:C:39:ARG:HD3	2.26	0.70
2:B:52:THR:HG22	3:C:191:THR:HG22	1.75	0.69
1:A:29:ASN:HB2	1:A:32:ARG:HD3	1.75	0.68
2:B:116:THR:CG2	3:C:235:THR:HG21	2.23	0.68
2:B:52:THR:HA	3:C:191:THR:HG21	1.75	0.67
4:D:16:ASN:O	4:D:17:GLU:HG2	1.95	0.67
3:C:189:GLN:O	3:C:192:THR:HG23	1.95	0.66
4:D:21:ILE:HD12	4:D:22:ASN:O	1.95	0.66
1:A:161:LEU:HB2	1:A:226:GLN:HE21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:THR:HG21	3:C:235:THR:CG2	2.26	0.65
1:A:84:PRO:O	1:A:222:ARG:NH2	2.30	0.64
3:C:68:ALA:HB2	3:C:80:ILE:CD1	2.28	0.64
2:B:58:ASP:HB2	2:B:62:LYS:O	1.97	0.63
2:B:84:THR:C	2:B:86:SER:H	2.07	0.63
3:C:68:ALA:HB2	3:C:80:ILE:HD12	1.81	0.63
2:B:51:PRO:O	3:C:191:THR:HG21	1.98	0.62
2:B:116:THR:HG21	3:C:235:THR:CB	2.29	0.62
2:B:116:THR:HG22	2:B:116:THR:O	2.00	0.61
2:B:114:VAL:HG22	2:B:158:SER:OG	2.00	0.60
1:A:222:ARG:HG3	5:A:400:HOH:O	2.01	0.59
2:B:83:VAL:CG2	2:B:185:ASP:HB3	2.33	0.59
2:B:84:THR:HG21	2:B:176:TYR:HE2	1.67	0.59
1:A:216:PRO:HB2	5:A:301:HOH:O	2.02	0.59
3:C:133:GLU:OE2	3:C:224:HIS:HE1	1.86	0.58
3:C:141:THR:HG22	3:C:142:GLU:N	2.18	0.58
3:C:250:THR:HG22	3:C:251:ALA:N	2.16	0.58
2:B:83:VAL:HG23	2:B:83:VAL:O	2.04	0.58
1:A:4:ASN:HD21	2:B:156:ASN:HA	1.69	0.57
3:C:34:PHE:HE1	3:C:39:ARG:HD3	1.69	0.57
3:C:141:THR:CG2	3:C:143:VAL:HG23	2.34	0.57
1:A:120:LYS:HE3	2:B:31:SER:OG	2.04	0.57
1:A:243:PHE:CD1	2:B:40:GLU:HB2	2.39	0.57
1:A:67:SER:HB2	1:A:224:LEU:HD22	1.86	0.57
2:B:51:PRO:O	3:C:191:THR:CG2	2.53	0.56
1:A:161:LEU:H	1:A:226:GLN:NE2	2.03	0.56
2:B:11:ALA:HB3	5:B:305:HOH:O	2.04	0.56
3:C:71:THR:H	3:C:74:GLN:HE21	1.50	0.56
1:A:247:PRO:HA	3:C:189:GLN:HE21	1.70	0.56
1:A:111:ILE:HG22	1:A:112:MET:HE2	1.88	0.55
1:A:234:HIS:HD2	5:A:325:HOH:O	1.87	0.55
2:B:79:VAL:CG2	2:B:190:VAL:HG13	2.37	0.55
2:B:58:ASP:HB3	2:B:62:LYS:H	1.73	0.54
2:B:104:GLN:HE22	2:B:221:ARG:NH2	2.03	0.54
2:B:84:THR:HG23	2:B:183:SER:O	2.08	0.53
2:B:222:MET:O	2:B:224:VAL:HG13	2.07	0.53
3:C:78:ASP:OD1	3:C:160:HIS:HD2	1.91	0.53
3:C:170:VAL:HG21	3:C:174:THR:HG21	1.90	0.53
1:A:45:VAL:HG13	1:A:64:LEU:HD22	1.89	0.53
3:C:115:GLN:OE1	3:C:250:THR:HG22	2.08	0.53
2:B:83:VAL:HG23	2:B:185:ASP:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LEU:HB2	1:A:226:GLN:NE2	2.24	0.52
3:C:68:ALA:CB	3:C:80:ILE:HD12	2.39	0.52
1:A:6:GLU:OE2	2:B:157:SER:OG	2.27	0.51
1:A:247:PRO:HA	3:C:189:GLN:NE2	2.25	0.51
2:B:84:THR:C	2:B:86:SER:N	2.68	0.51
2:B:138:LYS:N	2:B:142:GLN:HE21	2.06	0.51
3:C:250:THR:CG2	3:C:251:ALA:N	2.73	0.51
2:B:116:THR:HB	2:B:207:HIS:O	2.09	0.51
2:B:188:LEU:C	2:B:188:LEU:HD23	2.35	0.51
1:A:6:GLU:HA	3:C:197:ILE:HB	1.91	0.51
2:B:116:THR:HG21	3:C:235:THR:HB	1.92	0.51
3:C:171:ASN:ND2	3:C:173:THR:H	2.10	0.50
2:B:208:ILE:HD12	2:B:208:ILE:N	2.27	0.50
3:C:141:THR:HG22	3:C:143:VAL:HG23	1.94	0.49
1:A:29:ASN:O	1:A:32:ARG:HD3	2.12	0.49
1:A:72:PRO:O	1:A:111:ILE:HD11	2.11	0.49
3:C:264:ARG:HG3	3:C:264:ARG:HH11	1.78	0.49
2:B:50:ILE:HG21	3:C:192:THR:HA	1.95	0.49
4:D:15:GLY:O	4:D:16:ASN:CB	2.58	0.49
2:B:52:THR:HG22	3:C:191:THR:CG2	2.42	0.49
2:B:116:THR:CG2	2:B:116:THR:O	2.60	0.49
1:A:243:PHE:CE1	2:B:40:GLU:HB2	2.48	0.48
2:B:19:PRO:O	4:D:17:GLU:HA	2.13	0.48
1:A:204:SER:HB2	1:A:216:PRO:HB3	1.95	0.48
1:A:120:LYS:HE2	2:B:34:PHE:CD1	2.49	0.47
1:A:24:VAL:HG22	2:B:106:ARG:NH2	2.29	0.47
1:A:29:ASN:HB2	1:A:32:ARG:CD	2.44	0.47
1:A:74:PRO:HA	1:A:106:GLN:HB3	1.97	0.47
4:D:15:GLY:O	4:D:16:ASN:HB3	2.14	0.47
1:A:67:SER:HB2	1:A:224:LEU:CD2	2.44	0.47
3:C:257:LYS:HE2	5:C:349:HOH:O	2.15	0.47
1:A:208:ASN:O	3:C:146:ARG:NH2	2.48	0.46
1:A:225:LEU:C	1:A:225:LEU:HD23	2.41	0.46
2:B:85:LEU:HD12	2:B:174:THR:HG22	1.97	0.46
1:A:46:LEU:HD11	1:A:67:SER:N	2.31	0.46
1:A:46:LEU:HD11	1:A:67:SER:CA	2.45	0.46
3:C:196:GLN:NE2	3:C:207:ASP:H	2.13	0.46
1:A:111:ILE:HD12	1:A:111:ILE:N	2.31	0.46
2:B:52:THR:HA	3:C:191:THR:CG2	2.42	0.45
3:C:141:THR:HG22	3:C:143:VAL:H	1.82	0.45
1:A:34:SER:O	1:A:38:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:SER:O	3:C:77:PHE:HB2	2.17	0.45
1:A:74:PRO:HA	1:A:105:LYS:O	2.17	0.45
4:D:16:ASN:C	4:D:17:GLU:HG2	2.42	0.45
1:A:248:THR:CG2	1:A:249:VAL:N	2.79	0.45
3:C:82:VAL:HB	3:C:229:LEU:HB3	1.98	0.45
3:C:113:GLN:HA	3:C:206:CYS:O	2.16	0.45
3:C:72:LYS:HE3	3:C:239:TYR:CZ	2.52	0.45
3:C:213:VAL:O	3:C:214:ASN:HB2	2.17	0.45
2:B:77:PRO:HD3	2:B:191:TRP:CH2	2.52	0.45
2:B:104:GLN:NE2	2:B:221:ARG:HH21	2.06	0.45
3:C:43:LYS:O	3:C:107:LYS:HE2	2.17	0.44
3:C:110:TRP:O	3:C:209:GLU:HA	2.17	0.44
1:A:90:ILE:HG12	1:A:104:THR:HG21	1.99	0.44
1:A:60:THR:HG23	1:A:65:GLN:HE21	1.83	0.43
3:C:171:ASN:HD22	3:C:173:THR:H	1.66	0.43
2:B:207:HIS:HD2	3:C:235:THR:HG23	1.83	0.43
3:C:86:HIS:CD2	3:C:86:HIS:H	2.36	0.43
1:A:94:SER:HA	1:A:95:PRO:HD3	1.87	0.43
3:C:141:THR:CG2	3:C:142:GLU:N	2.82	0.43
3:C:139:HIS:HD2	5:C:392:HOH:O	2.02	0.42
2:B:31:SER:O	2:B:32:THR:C	2.62	0.42
1:A:116:PHE:C	1:A:246:ARG:HG2	2.44	0.42
2:B:11:ALA:N	5:B:301:HOH:O	2.52	0.42
2:B:100:ARG:HD2	2:B:226:PHE:CD1	2.54	0.42
2:B:104:GLN:HE21	2:B:221:ARG:HE	1.66	0.42
1:A:91:SER:HB2	1:A:103:LYS:HD3	2.01	0.42
3:C:101:ARG:HB3	3:C:267:VAL:HG22	2.01	0.42
1:A:90:ILE:HG23	1:A:104:THR:CG2	2.50	0.42
4:D:16:ASN:C	4:D:17:GLU:CG	2.93	0.42
2:B:83:VAL:CG2	2:B:83:VAL:O	2.67	0.42
2:B:51:PRO:HA	2:B:213:SER:HB3	2.02	0.41
3:C:135:ASP:OD1	3:C:139:HIS:CE1	2.73	0.41
1:A:139:VAL:CG1	1:A:223:LEU:HD22	2.49	0.41
1:A:200:PHE:CG	1:A:215:ALA:HB2	2.56	0.41
3:C:141:THR:HG21	3:C:143:VAL:HG23	2.03	0.41
3:C:124:GLY:HA2	3:C:235:THR:HG22	2.02	0.41
3:C:216:CYS:HB2	3:C:217:PRO:HD2	2.03	0.41
3:C:267:VAL:O	3:C:268:VAL:HG22	2.21	0.41
3:C:130:MET:HG2	3:C:208:LEU:HD23	2.03	0.40
2:B:45:LEU:HD21	2:B:219:THR:HA	2.03	0.40
2:B:79:VAL:HG22	2:B:190:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ARG:HD2	3:C:209:GLU:OE2	2.22	0.40
3:C:103:HIS:CG	3:C:260:PHE:HB3	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	250/252 (99%)	238 (95%)	11 (4%)	1 (0%)	30	49
2	B	230/232 (99%)	220 (96%)	9 (4%)	1 (0%)	30	49
3	C	256/258 (99%)	247 (96%)	9 (4%)	0	100	100
4	D	22/24 (92%)	20 (91%)	1 (4%)	1 (4%)	2	2
All	All	758/766 (99%)	725 (96%)	30 (4%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	16	ASN
1	A	244	CYS
2	B	223	PRO

### 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	233/233 (100%)	231 (99%)	2 (1%)	70	87
2	B	206/206 (100%)	202 (98%)	4 (2%)	50	76
3	C	222/222 (100%)	217 (98%)	5 (2%)	44	72
4	D	21/21 (100%)	19 (90%)	2 (10%)	8	17
All	All	682/682 (100%)	669 (98%)	13 (2%)	50	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	248	THR
2	B	23	VAL
2	B	144	MET
2	B	178	THR
2	B	190	VAL
3	C	80	ILE
3	C	114	VAL
3	C	120	GLN
3	C	146	ARG
3	C	233	VAL
4	D	20	ILE
4	D	27	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	47	GLN
1	A	65	GLN
1	A	86	GLN
1	A	226	GLN
1	A	228	GLN
1	A	234	HIS
2	B	10	HIS
2	B	56	ASN
2	B	103	ASN
2	B	104	GLN
2	B	142	GLN
2	B	145	GLN
2	B	156	ASN

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Mol	Chain	Res	Type
2	B	170	HIS
2	B	173	GLN
2	B	207	HIS
3	C	25	ASN
3	C	38	GLN
3	C	74	GLN
3	C	86	HIS
3	C	113	GLN
3	C	120	GLN
3	C	138	ASN
3	C	160	HIS
3	C	171	ASN
3	C	189	GLN
3	C	196	GLN
3	C	223	GLN
3	C	224	HIS
3	C	265	HIS
4	D	16	ASN
4	D	27	ASN
4	D	30	GLN
4	D	38	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	17:GLU	C	18:GLY	N	1.19

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	252/252 (100%)	-0.71	0 100 100	19, 25, 41, 51	0
2	B	232/232 (100%)	-0.73	0 100 100	18, 24, 40, 55	0
3	C	258/258 (100%)	-0.67	0 100 100	19, 24, 49, 72	0
4	D	24/24 (100%)	-0.43	0 100 100	23, 40, 62, 64	0
All	All	766/766 (100%)	-0.69	0 100 100	18, 24, 46, 72	0

There are no RSRZ outliers to report.

### 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.