



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:14 AM GMT

PDB ID : 2WCT
Title : HUMAN SARS CORONAVIRUS UNIQUE DOMAIN (TRICLINIC FORM)
Authors : Tan, J.; Vonnrhein, C.; Smart, O.S.; Bricogne, G.; Bollati, M.; Hansen, G.;
Mesters, J.R.; Hilgenfeld, R.
Deposited on : 2009-03-16
Resolution : 2.79 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

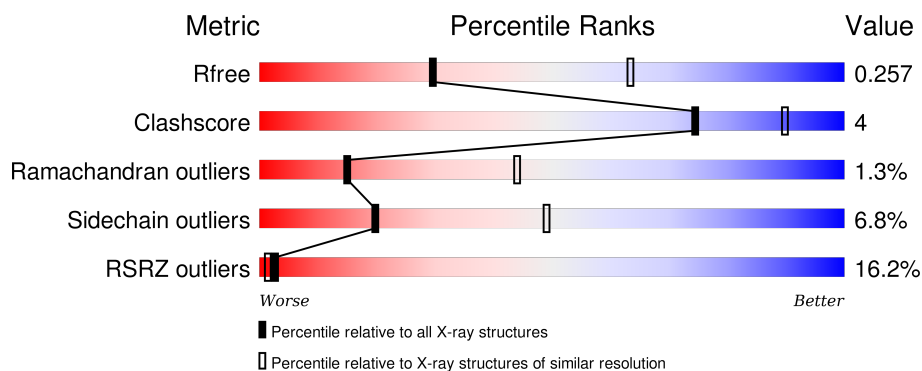
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	264	<div> <div>15%</div> <div>80%</div> <div>16%</div> <div>• •</div> </div>
1	B	264	<div> <div>16%</div> <div>81%</div> <div>16%</div> <div>• •</div> </div>
1	C	264	<div> <div>16%</div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div>
1	D	264	<div> <div>15%</div> <div>78%</div> <div>15%</div> <div>• 6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7849 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 NON-STRUCTURAL PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1991	1268	326	381	16			
1	B	257	Total	C	N	O	S	0	0	0
			1991	1268	326	381	16			
1	C	252	Total	C	N	O	S	0	0	0
			1954	1246	321	371	16			
1	D	248	Total	C	N	O	S	0	0	0
			1908	1214	316	362	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	628	ARG	LYS	CONFLICT	UNP P0C6U8
B	628	ARG	LYS	CONFLICT	UNP P0C6U8
C	628	ARG	LYS	CONFLICT	UNP P0C6U8
D	628	ARG	LYS	CONFLICT	UNP P0C6U8

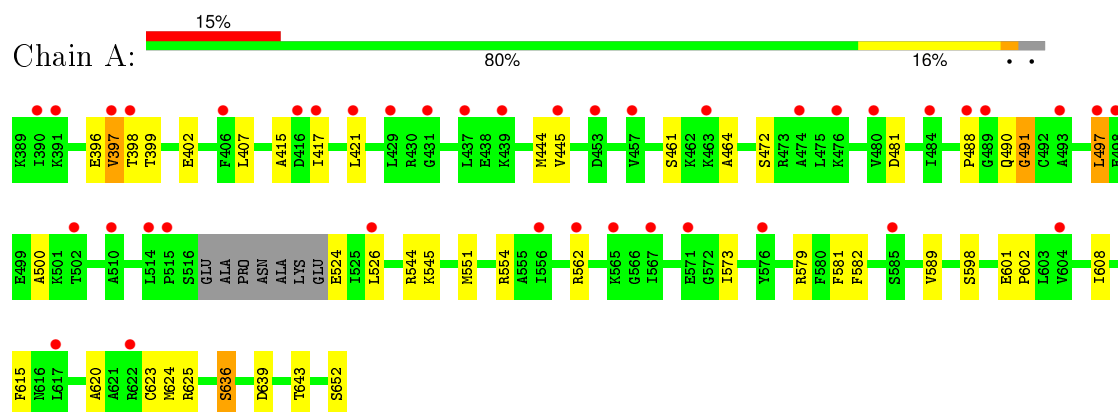
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	C	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		

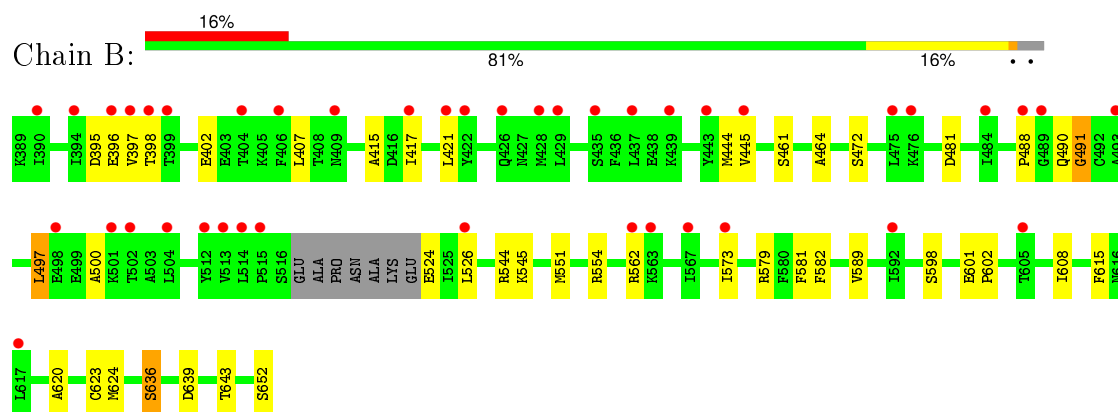
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

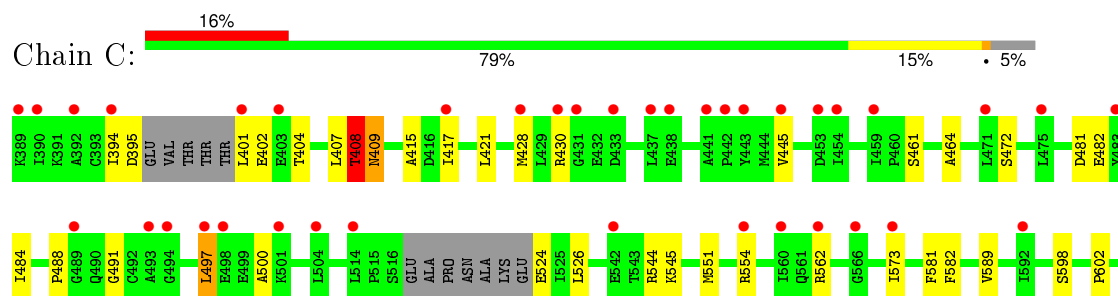
• Molecule 1: NON-STRUCTURAL PROTEIN 3

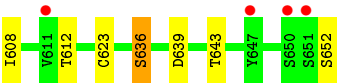


• Molecule 1: NON-STRUCTURAL PROTEIN 3

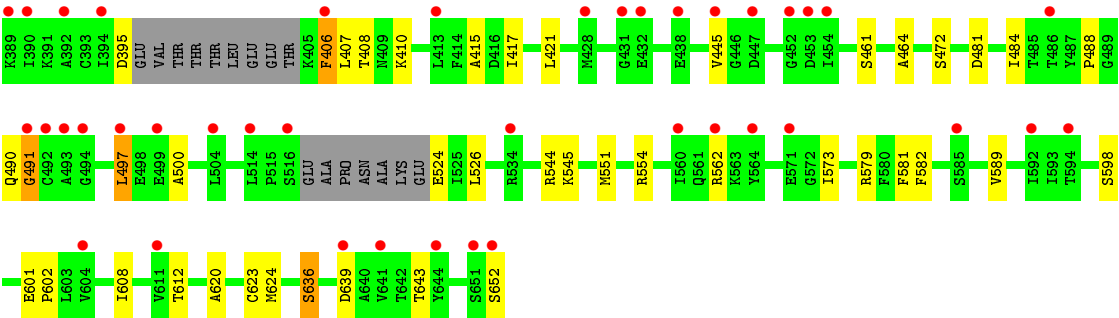
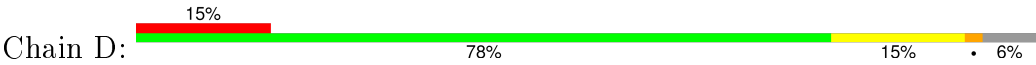


• Molecule 1: NON-STRUCTURAL PROTEIN 3





● Molecule 1: NON-STRUCTURAL PROTEIN 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.68Å 75.52Å 80.54Å 77.16° 75.61° 74.48°	Depositor
Resolution (Å)	33.33 – 2.79 33.33 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (33.33-2.79) 72.2 (33.33-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT 2.7.0	Depositor
R, R_{free}	0.223 , 0.240 0.240 , 0.257	Depositor DCC
R_{free} test set	1652 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 33106 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7849	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.50	0/2025	0.70	0/2736
1	B	0.51	0/2025	0.71	0/2736
1	C	0.49	0/1987	0.73	1/2681 (0.0%)
1	D	0.49	0/1940	0.72	0/2619
All	All	0.49	0/7977	0.71	1/10772 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	408	THR	C-N-CA	6.26	137.34	121.70

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	1991	0	2031	17	0
1	B	1991	0	2031	15	0
1	C	1954	0	1994	18	0
1	D	1908	0	1937	16	0
2	A	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	7849	0	7993	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (64) 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:394:ILE:HG12	1:C:404:THR:HG21	1.50	0.93
1:D:497:LEU:H	1:D:652:SER:HB3	1.61	0.64
1:A:497:LEU:H	1:A:652:SER:HB3	1.63	0.64
1:C:497:LEU:H	1:C:652:SER:HB3	1.62	0.63
1:D:408:THR:HG23	1:D:484:ILE:HD11	1.80	0.62
1:D:417:ILE:HD11	1:D:445:VAL:HG23	1.82	0.61
1:C:417:ILE:HD11	1:C:445:VAL:HG23	1.82	0.60
1:B:497:LEU:H	1:B:652:SER:HB3	1.67	0.60
1:A:417:ILE:HD11	1:A:445:VAL:HG23	1.82	0.60
1:B:417:ILE:HD11	1:B:445:VAL:HG23	1.84	0.59
1:C:394:ILE:HG12	1:C:404:THR:CG2	2.32	0.55
1:C:408:THR:HA	1:C:409:ASN:HB2	1.90	0.54
1:C:401:LEU:HD23	1:C:430:ARG:HE	1.73	0.53
1:A:545:LYS:HG2	1:A:602:PRO:HB2	1.95	0.49
1:B:545:LYS:HG2	1:B:602:PRO:HB2	1.95	0.48
1:C:401:LEU:HD21	1:C:428:MET:O	2.13	0.48
1:C:408:THR:HG23	1:C:484:ILE:HD11	1.96	0.47
1:D:406:PHE:HA	1:D:407:LEU:HA	1.56	0.47
1:D:545:LYS:HG2	1:D:602:PRO:HB2	1.96	0.47
1:C:545:LYS:HG2	1:C:602:PRO:HB2	1.97	0.47
1:D:488:PRO:HD2	1:D:500:ALA:HB1	1.98	0.46
1:C:488:PRO:HD2	1:C:500:ALA:HB1	1.99	0.45
1:C:408:THR:O	1:C:484:ILE:HD11	2.16	0.45
1:B:415:ALA:HB2	1:B:421:LEU:HD23	1.98	0.45
1:A:415:ALA:HB2	1:A:421:LEU:HD23	1.99	0.45
1:A:551:MET:HG3	1:A:582:PHE:HB3	1.99	0.45
1:C:461:SER:HB3	1:C:464:ALA:HB3	1.99	0.45
1:C:415:ALA:HB2	1:C:421:LEU:HD23	1.98	0.45
1:A:488:PRO:HD2	1:A:500:ALA:HB1	1.98	0.44
1:D:415:ALA:HB2	1:D:421:LEU:HD23	1.98	0.44
1:C:551:MET:HG3	1:C:582:PHE:HB3	1.99	0.44
1:B:551:MET:HG3	1:B:582:PHE:HB3	2.00	0.44
1:B:573:ILE:HD13	1:B:581:PHE:HD1	1.83	0.44
1:B:461:SER:HB3	1:B:464:ALA:HB3	1.99	0.44
1:D:461:SER:HB3	1:D:464:ALA:HB3	1.99	0.44
1:C:573:ILE:HD13	1:C:581:PHE:HD1	1.83	0.44
1:D:573:ILE:HD13	1:D:581:PHE:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:GLN:HA	1:D:491:GLY:HA2	1.80	0.43
1:A:573:ILE:HD13	1:A:581:PHE:HD1	1.83	0.43
1:D:551:MET:HG3	1:D:582:PHE:HB3	1.99	0.43
1:B:490:GLN:HA	1:B:491:GLY:HA2	1.85	0.43
1:B:488:PRO:HD2	1:B:500:ALA:HB1	2.00	0.43
1:C:589:VAL:HG13	1:C:608:ILE:HG22	2.01	0.42
1:A:461:SER:HB3	1:A:464:ALA:HB3	2.01	0.42
1:B:589:VAL:HG21	1:B:615:PHE:CE2	2.55	0.42
1:A:490:GLN:HA	1:A:491:GLY:HA2	1.84	0.42
1:A:579:ARG:NH1	1:A:601:GLU:OE2	2.53	0.42
1:B:579:ARG:NH1	1:B:601:GLU:OE2	2.53	0.41
1:D:589:VAL:HG13	1:D:608:ILE:HG22	2.02	0.41
1:A:625:ARG:HH12	1:A:652:SER:HB2	1.86	0.41
1:A:524:GLU:HG3	1:A:526:LEU:H	1.85	0.41
1:B:524:GLU:HG3	1:B:526:LEU:H	1.86	0.41
1:A:589:VAL:HG13	1:A:608:ILE:HG22	2.03	0.41
1:B:620:ALA:O	1:B:624:MET:HG2	2.20	0.41
1:A:620:ALA:O	1:A:624:MET:HG2	2.21	0.41
1:D:524:GLU:HG3	1:D:526:LEU:H	1.85	0.41
1:A:397:VAL:HA	1:A:398:THR:HA	1.80	0.41
1:A:589:VAL:HG21	1:A:615:PHE:CE2	2.56	0.40
1:B:444:MET:HG2	1:C:612:THR:HA	2.03	0.40
1:A:444:MET:HG2	1:D:612:THR:HA	2.03	0.40
1:C:524:GLU:HG3	1:C:526:LEU:H	1.86	0.40
1:D:620:ALA:O	1:D:624:MET:HG2	2.21	0.40
1:B:589:VAL:HG13	1:B:608:ILE:HG22	2.04	0.40
1:D:579:ARG:NH1	1:D:601:GLU:OE2	2.52	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	253/264 (96%)	239 (94%)	12 (5%)	2 (1%)	24	58
1	B	253/264 (96%)	238 (94%)	12 (5%)	3 (1%)	16	47
1	C	246/264 (93%)	232 (94%)	10 (4%)	4 (2%)	12	38
1	D	242/264 (92%)	227 (94%)	11 (4%)	4 (2%)	11	36
All	All	994/1056 (94%)	936 (94%)	45 (4%)	13 (1%)	15	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	409	ASN
1	A	636	SER
1	D	406	PHE
1	D	410	LYS
1	B	398	THR
1	B	636	SER
1	C	408	THR
1	C	636	SER
1	D	636	SER
1	A	491	GLY
1	B	491	GLY
1	C	491	GLY
1	D	491	GLY

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	222/227 (98%)	206 (93%)	16 (7%)	18	45
1	B	222/227 (98%)	206 (93%)	16 (7%)	18	45
1	C	217/227 (96%)	202 (93%)	15 (7%)	19	48
1	D	210/227 (92%)	198 (94%)	12 (6%)	25	58
All	All	871/908 (96%)	812 (93%)	59 (7%)	20	49

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	396	GLU
1	A	397	VAL
1	A	399	THR
1	A	402	GLU
1	A	407	LEU
1	A	472	SER
1	A	481	ASP
1	A	497	LEU
1	A	544	ARG
1	A	554	ARG
1	A	562	ARG
1	A	598	SER
1	A	623	CYS
1	A	636	SER
1	A	639	ASP
1	A	643	THR
1	B	395	ASP
1	B	396	GLU
1	B	397	VAL
1	B	402	GLU
1	B	407	LEU
1	B	472	SER
1	B	481	ASP
1	B	497	LEU
1	B	544	ARG
1	B	554	ARG
1	B	562	ARG
1	B	598	SER
1	B	623	CYS
1	B	636	SER
1	B	639	ASP
1	B	643	THR
1	C	395	ASP
1	C	402	GLU
1	C	407	LEU
1	C	472	SER
1	C	481	ASP
1	C	482	GLU
1	C	497	LEU
1	C	544	ARG
1	C	554	ARG
1	C	562	ARG
1	C	598	SER

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Mol	Chain	Res	Type
1	C	623	CYS
1	C	636	SER
1	C	639	ASP
1	C	643	THR
1	D	395	ASP
1	D	472	SER
1	D	481	ASP
1	D	497	LEU
1	D	544	ARG
1	D	554	ARG
1	D	562	ARG
1	D	598	SER
1	D	623	CYS
1	D	636	SER
1	D	639	ASP
1	D	643	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	409	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

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	257/264 (97%)	1.06	40 (15%) 3 1	44, 69, 109, 127	0
1	B	257/264 (97%)	1.11	42 (16%) 2 1	46, 75, 114, 124	0
1	C	252/264 (95%)	1.21	42 (16%) 2 1	47, 74, 106, 124	0
1	D	248/264 (93%)	1.15	40 (16%) 3 1	46, 78, 108, 131	0
All	All	1014/1056 (96%)	1.13	164 (16%) 3 1	44, 74, 110, 131	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	LYS	6.7
1	D	651	SER	6.2
1	D	494	GLY	5.6
1	C	431	GLY	5.6
1	D	389	LYS	5.4
1	B	398	THR	5.2
1	C	443	TYR	4.9
1	D	491	GLY	4.5
1	D	406	PHE	4.5
1	B	397	VAL	4.4
1	A	488	PRO	4.3
1	B	439	LYS	4.3
1	D	431	GLY	4.2
1	B	513	VAL	4.2
1	A	493	ALA	4.0
1	C	562	ARG	4.0
1	C	401	LEU	3.9
1	C	494	GLY	3.9
1	D	486	THR	3.9
1	C	453	ASP	3.9
1	B	488	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	652	SER	3.9
1	B	493	ALA	3.8
1	D	390	ILE	3.7
1	B	443	TYR	3.7
1	C	651	SER	3.7
1	B	394	ILE	3.6
1	C	504	LEU	3.6
1	A	562	ARG	3.6
1	A	398	THR	3.6
1	C	454	ILE	3.6
1	B	445	VAL	3.6
1	C	514	LEU	3.6
1	D	497	LEU	3.5
1	A	437	LEU	3.5
1	A	489	GLY	3.4
1	C	441	ALA	3.4
1	C	497	LEU	3.4
1	D	492	CYS	3.3
1	B	435	SER	3.3
1	A	476	LYS	3.3
1	A	390	ILE	3.2
1	C	493	ALA	3.2
1	D	514	LEU	3.1
1	B	409	ASN	3.1
1	C	394	ILE	3.1
1	B	390	ILE	3.0
1	D	394	ILE	3.0
1	D	560	ILE	3.0
1	C	417	ILE	3.0
1	D	611	VAL	2.9
1	A	406	PHE	2.9
1	A	429	LEU	2.9
1	D	453	ASP	2.9
1	D	392	ALA	2.9
1	A	416	ASP	2.9
1	D	493	ALA	2.8
1	D	592	ILE	2.8
1	A	439	LYS	2.8
1	C	428	MET	2.8
1	C	554	ARG	2.8
1	B	484	ILE	2.8
1	B	515	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	459	ILE	2.7
1	D	432	GLU	2.7
1	D	413	LEU	2.7
1	B	562	ARG	2.7
1	D	452	GLY	2.7
1	A	604	VAL	2.7
1	A	445	VAL	2.6
1	C	445	VAL	2.6
1	D	428	MET	2.6
1	C	430	ARG	2.6
1	D	504	LEU	2.6
1	B	426	GLN	2.6
1	C	566	GLY	2.6
1	A	463	LYS	2.6
1	A	502	THR	2.5
1	B	498	GLU	2.5
1	A	397	VAL	2.5
1	C	592	ILE	2.5
1	C	611	VAL	2.5
1	A	480	VAL	2.5
1	D	594	THR	2.5
1	A	453	ASP	2.5
1	B	399	THR	2.5
1	A	431	GLY	2.5
1	D	499	GLU	2.4
1	C	390	ILE	2.4
1	B	605	THR	2.4
1	B	428	MET	2.4
1	B	476	LYS	2.4
1	C	647	TYR	2.4
1	C	438	GLU	2.4
1	B	429	LEU	2.4
1	C	442	PRO	2.4
1	B	396	GLU	2.4
1	B	514	LEU	2.4
1	D	562	ARG	2.4
1	A	571	GLU	2.3
1	B	422	TYR	2.3
1	D	564	TYR	2.3
1	B	501	LYS	2.3
1	D	438	GLU	2.3
1	D	454	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	489	GLY	2.3
1	C	498	GLU	2.2
1	C	650	SER	2.2
1	B	417	ILE	2.2
1	A	474	ALA	2.2
1	C	573	ILE	2.2
1	B	504	LEU	2.2
1	A	510	ALA	2.2
1	D	445	VAL	2.2
1	A	417	ILE	2.2
1	A	498	GLU	2.2
1	A	515	PRO	2.2
1	A	421	LEU	2.2
1	B	421	LEU	2.2
1	B	563	LYS	2.2
1	A	622	ARG	2.2
1	D	534	ARG	2.2
1	C	542	GLU	2.1
1	C	501	LYS	2.1
1	D	641	VAL	2.1
1	C	489	GLY	2.1
1	A	526	LEU	2.1
1	B	437	LEU	2.1
1	B	526	LEU	2.1
1	C	437	LEU	2.1
1	C	475	LEU	2.1
1	D	516	SER	2.1
1	B	592	ILE	2.1
1	C	560	ILE	2.1
1	D	571	GLU	2.1
1	A	497	LEU	2.1
1	B	617	LEU	2.1
1	C	403	GLU	2.1
1	D	644	TYR	2.1
1	A	391	LYS	2.1
1	A	585	SER	2.1
1	B	502	THR	2.1
1	D	604	VAL	2.1
1	A	484	ILE	2.1
1	A	567	ILE	2.1
1	B	567	ILE	2.1
1	B	573	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	392	ALA	2.1
1	A	514	LEU	2.1
1	D	585	SER	2.1
1	A	565	LYS	2.1
1	C	483	TYR	2.1
1	B	475	LEU	2.0
1	D	639	ASP	2.0
1	A	576	TYR	2.0
1	B	512	TYR	2.0
1	B	406	PHE	2.0
1	A	617	LEU	2.0
1	C	471	LEU	2.0
1	A	457	VAL	2.0
1	A	556	ILE	2.0
1	D	447	ASP	2.0
1	B	404	THR	2.0
1	C	433	ASP	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 carbohydrates 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.