



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:01 PM EDT

PDB ID : 4E68 / pdb\_00004e68  
Title : Unphosphorylated STAT3B core protein binding to dsDNA  
Authors : Collie, G.W.; Parkinson, G.N.; Shah, R.  
Deposited on : 2012-03-15  
Resolution : 2.58 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

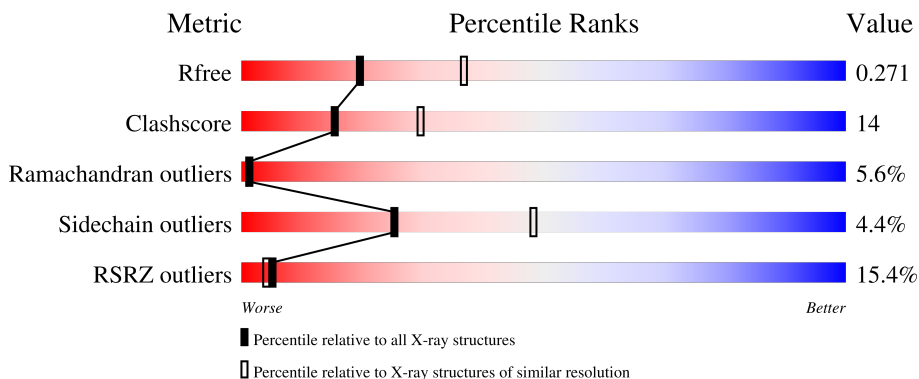
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	B	18	
2	A	596	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4998 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 DNA chain called DNA (5'-D(\*TP\*GP\*CP\*AP\*TP\*TP\*TP\*CP\*CP\*CP\*GP\*TP\*AP\*AP\*AP\*TP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	18	360	175	59	109	17	0	0	0

- Molecule 2 is a protein called Signal transducer and activator of transcription 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	559	4499	2869	766	834	30	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	631	SER	LYS	conflict	UNP P42227

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	24	Total 24	O 24	0	0
3	A	115	Total 115	O 115	0	0

### 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.

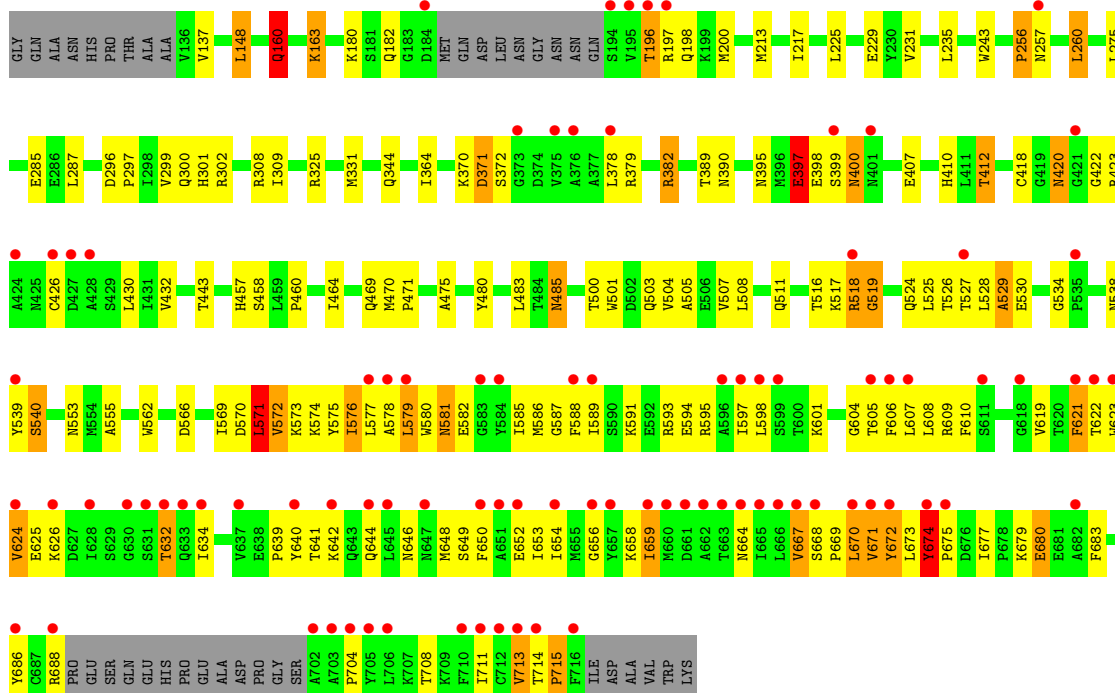
- Molecule 1: DNA (5'-D(\*TP\*GP\*CP\*AP\*TP\*TP\*TP\*CP\*CP\*CP\*GP\*TP\*AP\*AP\*AP\*TP\*CP\*T)-3')

Chain B:  72% 28%



- Molecule 2: Signal transducer and activator of transcription 3

Chain A:  15% 64% 24% 5% • 6%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.14Å 174.14Å 79.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.58 14.98 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.1 (14.98-2.58) 97.1 (14.98-2.58)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.225 , 0.273 0.224 , 0.271	Depositor DCC
$R_{free}$ test set	1811 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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	B	0.35	0/401	1.12	1/616 (0.2%)
2	A	0.75	0/4586	1.14	24/6194 (0.4%)
All	All	0.73	0/4987	1.14	25/6810 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	198	GLN	N-CA-C	-10.48	100.50	113.18
2	A	389	THR	CA-C-N	8.61	132.69	120.28
2	A	389	THR	C-N-CA	8.61	132.69	120.28
2	A	200	MET	N-CA-C	-7.75	102.84	111.28
2	A	483	LEU	N-CA-C	7.50	123.34	113.30
2	A	390	ASN	N-CA-CB	-7.49	98.69	110.22
2	A	708	THR	N-CA-C	6.59	119.20	109.24
2	A	160	GLN	N-CA-C	-6.29	104.34	111.07
2	A	624	VAL	N-CA-C	6.27	117.77	106.61
2	A	621	PHE	N-CA-C	6.25	116.32	108.45
2	A	382	ARG	N-CA-C	-6.22	102.32	110.53
1	B	1012	DT	P-O3'-C3'	6.20	129.49	120.20
2	A	674	TYR	N-CA-C	6.00	123.07	109.81
2	A	518	ARG	N-CA-C	5.85	117.74	108.79
2	A	137	VAL	N-CA-C	5.80	116.50	108.84
2	A	601	LYS	CA-C-N	5.78	123.82	119.66
2	A	601	LYS	C-N-CA	5.78	123.82	119.66
2	A	529	ALA	N-CA-C	-5.65	105.65	112.54
2	A	516	THR	N-CA-C	5.55	117.06	109.18
2	A	516	THR	CA-C-N	5.47	127.61	120.28
2	A	516	THR	C-N-CA	5.47	127.61	120.28
2	A	652	GLU	N-CA-C	-5.46	105.35	112.23
2	A	585	ILE	N-CA-C	5.23	116.25	108.46
2	A	674	TYR	CA-C-N	-5.22	113.32	119.84
2	A	674	TYR	C-N-CA	-5.22	113.32	119.84

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	B	360	0	207	2	0
2	A	4499	0	4554	128	0
3	A	115	0	0	7	0
3	B	24	0	0	0	0
All	All	4998	0	4761	130	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 14.

All (130) 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:A:597:ILE:HG13	2:A:598:LEU:H	1.13	1.07
2:A:597:ILE:HD11	2:A:622:THR:HG21	1.51	0.92
2:A:672:TYR:HA	2:A:677:ILE:O	1.77	0.84
2:A:524:GLN:HG2	2:A:586:MET:O	1.78	0.83
2:A:597:ILE:HG13	2:A:598:LEU:N	1.90	0.81
2:A:196:THR:HG23	3:A:808:HOH:O	1.88	0.73
2:A:669:PRO:HG2	2:A:679:LYS:HE3	1.71	0.72
2:A:370:LYS:O	2:A:372:SER:N	2.24	0.69
2:A:576:ILE:HG22	2:A:576:ILE:O	1.91	0.69
2:A:569:ILE:O	2:A:572:VAL:HG12	1.95	0.67
2:A:640:TYR:HB3	2:A:644:GLN:HB2	1.76	0.67
2:A:668:SER:HB2	2:A:669:PRO:HD2	1.75	0.67
2:A:518:ARG:HG2	2:A:519:GLY:N	2.09	0.67
2:A:604:GLY:HA2	2:A:670:LEU:HB3	1.76	0.67
2:A:587:GLY:HA2	2:A:609:ARG:HA	1.77	0.66
2:A:395:ASN:OD1	2:A:397:GLU:HB2	1.95	0.66
2:A:518:ARG:HG2	2:A:519:GLY:H	1.61	0.66
2:A:578:ALA:O	2:A:581:ASN:HB3	1.96	0.65
2:A:412:THR:HB	3:A:831:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:430:LEU:HA	3:A:908:HOH:O	1.95	0.65
2:A:586:MET:HG3	2:A:607:LEU:HG	1.78	0.65
2:A:604:GLY:HA2	2:A:670:LEU:HD12	1.79	0.65
1:B:1017:DC:H1'	1:B:1018:DT:H5'	1.79	0.65
2:A:485:ASN:H	2:A:485:ASN:HD22	1.45	0.64
2:A:597:ILE:CG1	2:A:598:LEU:H	2.01	0.64
2:A:575:TYR:HE2	2:A:646:ASN:ND2	1.96	0.63
2:A:382:ARG:CZ	2:A:432:VAL:CG2	2.77	0.63
2:A:575:TYR:HE2	2:A:646:ASN:HD21	1.46	0.62
2:A:572:VAL:O	2:A:572:VAL:HG13	2.00	0.61
2:A:597:ILE:CD1	2:A:622:THR:HG21	2.29	0.61
2:A:229:GLU:OE2	2:A:308:ARG:HD2	2.01	0.60
2:A:530:GLU:O	2:A:534:GLY:N	2.30	0.60
2:A:285:GLU:HB2	2:A:302:ARG:HD2	1.85	0.58
2:A:605:THR:HG22	2:A:672:TYR:HB2	1.86	0.58
2:A:163:LYS:HE3	2:A:163:LYS:HA	1.86	0.57
2:A:501:TRP:CZ2	2:A:529:ALA:HB2	2.40	0.56
2:A:598:LEU:HD13	2:A:624:VAL:HG13	1.87	0.56
2:A:378:LEU:HD11	3:A:909:HOH:O	2.05	0.56
2:A:658:LYS:C	2:A:659:ILE:HD12	2.32	0.55
2:A:457:HIS:HD2	2:A:458:SER:O	1.89	0.55
2:A:243:TRP:CE2	2:A:260:LEU:HD11	2.41	0.54
1:B:1001:DT:H2''	1:B:1002:DG:C8	2.42	0.54
2:A:605:THR:HA	2:A:672:TYR:O	2.08	0.54
2:A:640:TYR:HB3	2:A:644:GLN:CB	2.37	0.54
2:A:648:MET:HE1	2:A:711:ILE:HG12	1.90	0.54
2:A:679:LYS:O	2:A:680:GLU:HB2	2.08	0.54
2:A:160:GLN:HE21	2:A:160:GLN:HA	1.72	0.53
2:A:527:THR:OG1	2:A:588:PHE:O	2.24	0.53
2:A:658:LYS:HA	2:A:668:SER:HA	1.91	0.53
2:A:604:GLY:O	2:A:670:LEU:HB3	2.08	0.53
2:A:371:ASP:OD1	2:A:372:SER:N	2.42	0.53
2:A:504:VAL:O	2:A:508:LEU:HG	2.10	0.52
2:A:659:ILE:HD12	2:A:659:ILE:N	2.25	0.52
2:A:180:LYS:C	2:A:182:GLN:H	2.18	0.52
2:A:296:ASP:O	2:A:299:VAL:HG22	2.11	0.51
2:A:505:ALA:HB1	2:A:525:LEU:HD21	1.93	0.51
2:A:650:PHE:O	2:A:654:ILE:HG13	2.10	0.51
2:A:470:MET:HB3	2:A:471:PRO:HD3	1.93	0.51
2:A:344:GLN:OE1	2:A:410:HIS:ND1	2.44	0.50
2:A:500:THR:OG1	2:A:503:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:571:LEU:C	2:A:573:LYS:H	2.19	0.50
2:A:160:GLN:HA	2:A:160:GLN:NE2	2.27	0.49
2:A:622:THR:HG23	2:A:634:ILE:HG23	1.94	0.49
2:A:382:ARG:CZ	2:A:432:VAL:HG23	2.42	0.49
2:A:243:TRP:CE2	2:A:260:LEU:CD1	2.96	0.49
2:A:460:PRO:HG2	2:A:480:TYR:CZ	2.48	0.49
2:A:619:VAL:O	3:A:824:HOH:O	2.20	0.49
2:A:649:SER:O	2:A:653:ILE:HG13	2.12	0.49
2:A:679:LYS:O	2:A:679:LYS:HG3	2.12	0.49
2:A:639:PRO:HA	3:A:824:HOH:O	2.12	0.48
2:A:300:GLN:HG3	2:A:301:HIS:CD2	2.49	0.48
2:A:591:LYS:HA	2:A:594:GLU:HB3	1.96	0.48
2:A:576:ILE:HD11	2:A:619:VAL:HG21	1.95	0.47
2:A:594:GLU:O	2:A:597:ILE:HG12	2.14	0.47
2:A:624:VAL:HG11	2:A:632:THR:HB	1.96	0.47
2:A:579:LEU:H	2:A:579:LEU:CD1	2.27	0.47
2:A:658:LYS:O	2:A:713:VAL:HG13	2.15	0.47
2:A:553:ASN:HD22	2:A:553:ASN:N	2.13	0.47
2:A:573:LYS:O	2:A:577:LEU:HB2	2.14	0.46
2:A:256:PRO:HB2	2:A:257:ASN:H	1.52	0.46
2:A:668:SER:HB2	2:A:669:PRO:CD	2.45	0.46
2:A:213:MET:O	2:A:217:ILE:HG13	2.15	0.46
2:A:679:LYS:O	2:A:680:GLU:CB	2.64	0.46
2:A:378:LEU:H	2:A:378:LEU:HD23	1.80	0.46
2:A:575:TYR:CE2	2:A:646:ASN:ND2	2.81	0.46
2:A:148:LEU:HD13	2:A:231:VAL:HG11	1.98	0.45
2:A:464:ILE:HB	2:A:469:GLN:OE1	2.17	0.45
2:A:579:LEU:HD12	2:A:579:LEU:N	2.32	0.45
2:A:507:VAL:O	2:A:511:GLN:HG2	2.16	0.45
2:A:539:TYR:O	2:A:540:SER:C	2.59	0.45
2:A:714:THR:HA	2:A:715:PRO:HD3	1.79	0.45
2:A:673:LEU:HD11	3:A:878:HOH:O	2.15	0.45
2:A:397:GLU:O	2:A:399:SER:N	2.50	0.44
2:A:525:LEU:O	2:A:528:LEU:HB3	2.17	0.44
2:A:572:VAL:CG2	2:A:580:TRP:HB2	2.47	0.44
2:A:604:GLY:O	2:A:671:VAL:O	2.35	0.44
2:A:485:ASN:HD22	2:A:485:ASN:N	2.09	0.44
2:A:325:ARG:NH2	2:A:407:GLU:OE2	2.51	0.44
2:A:517:LYS:NZ	2:A:577:LEU:O	2.50	0.43
2:A:581:ASN:ND2	2:A:686:TYR:OH	2.51	0.43
2:A:641:THR:O	2:A:642:LYS:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:382:ARG:NH1	2:A:432:VAL:CG2	2.81	0.43
2:A:595:ARG:HG2	2:A:634:ILE:HD12	2.00	0.43
2:A:607:LEU:O	2:A:621:PHE:HA	2.17	0.43
2:A:610:PHE:CD1	2:A:619:VAL:HG12	2.53	0.43
2:A:573:LYS:O	2:A:574:LYS:C	2.61	0.43
2:A:623:TRP:CZ3	2:A:659:ILE:HG12	2.53	0.43
2:A:667:VAL:HG12	2:A:668:SER:N	2.33	0.43
2:A:576:ILE:HG23	2:A:579:LEU:HB2	2.00	0.43
2:A:517:LYS:NZ	2:A:581:ASN:HA	2.34	0.43
2:A:399:SER:O	2:A:400:ASN:C	2.61	0.43
2:A:673:LEU:N	2:A:677:ILE:O	2.49	0.43
2:A:608:LEU:HD11	2:A:683:PHE:CZ	2.54	0.42
2:A:285:GLU:HB2	2:A:302:ARG:CD	2.49	0.42
2:A:309:ILE:HD12	2:A:309:ILE:HA	1.93	0.42
2:A:572:VAL:HG22	2:A:580:TRP:HB2	2.02	0.42
2:A:589:ILE:HD11	2:A:593:ARG:HG3	2.02	0.41
2:A:671:VAL:HA	2:A:679:LYS:HG2	2.02	0.41
2:A:670:LEU:HD22	2:A:670:LEU:N	2.35	0.41
2:A:562:TRP:CE2	2:A:566:ASP:HB2	2.55	0.41
2:A:606:PHE:O	2:A:674:TYR:N	2.46	0.41
2:A:650:PHE:HA	2:A:653:ILE:HD12	2.02	0.41
2:A:625:GLU:O	2:A:626:LYS:HB2	2.21	0.41
2:A:297:PRO:HA	2:A:300:GLN:HG2	2.03	0.41
2:A:526:THR:C	2:A:528:LEU:H	2.28	0.41
2:A:517:LYS:CE	2:A:581:ASN:HA	2.50	0.41
2:A:579:LEU:H	2:A:579:LEU:HD12	1.86	0.41
2:A:243:TRP:NE1	2:A:260:LEU:HD13	2.36	0.41
2:A:475:ALA:HB2	2:A:562:TRP:CD1	2.56	0.40
2:A:364:ILE:HD13	2:A:443:THR:HB	2.03	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
2	A	553/596 (93%)	468 (85%)	54 (10%)	31 (6%)	<b>1</b> <b>1</b>

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	256	PRO
2	A	371	ASP
2	A	398	GLU
2	A	400	ASN
2	A	581	ASN
2	A	582	GLU
2	A	664	ASN
2	A	667	VAL
2	A	674	TYR
2	A	680	GLU
2	A	704	PRO
2	A	420	ASN
2	A	426	CYS
2	A	540	SER
2	A	555	ALA
2	A	656	GLY
2	A	675	PRO
2	A	713	VAL
2	A	715	PRO
2	A	519	GLY
2	A	538	ASN
2	A	196	THR
2	A	570	ASP
2	A	571	LEU
2	A	572	VAL
2	A	397	GLU
2	A	418	CYS
2	A	632	THR
2	A	422	GLY
2	A	672	TYR
2	A	576	ILE

### 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
2	A	504/534 (94%)	482 (96%)	22 (4%)	25 48

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	148	LEU
2	A	160	GLN
2	A	163	LYS
2	A	197	ARG
2	A	225	LEU
2	A	235	LEU
2	A	260	LEU
2	A	275	LEU
2	A	287	LEU
2	A	331	MET
2	A	379	ARG
2	A	397	GLU
2	A	412	THR
2	A	420	ASN
2	A	423	ARG
2	A	485	ASN
2	A	571	LEU
2	A	579	LEU
2	A	659	ILE
2	A	670	LEU
2	A	671	VAL
2	A	688	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	149	GLN
2	A	160	GLN
2	A	167	ASN
2	A	288	GLN
2	A	301	HIS
2	A	332	HIS
2	A	420	ASN
2	A	425	ASN

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Mol	Chain	Res	Type
2	A	447	HIS
2	A	457	HIS
2	A	472	ASN
2	A	485	ASN
2	A	503	GLN
2	A	553	ASN
2	A	581	ASN
2	A	635	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](#)

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, 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	B	18/18 (100%)	-0.63	0 <b>100</b> <b>100</b>	38, 50, 70, 82	0
2	A	559/596 (93%)	0.44	89 (15%) <b>5</b> <b>4</b>	33, 62, 142, 172	0
All	All	577/614 (93%)	0.41	89 (15%) <b>5</b> <b>4</b>	33, 61, 140, 172	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	622	THR	7.6
2	A	195	VAL	6.6
2	A	605	THR	6.6
2	A	710	PHE	6.0
2	A	665	ILE	5.4
2	A	624	VAL	5.4
2	A	632	THR	5.2
2	A	711	ILE	5.1
2	A	668	SER	4.9
2	A	589	ILE	4.8
2	A	702	ALA	4.5
2	A	713	VAL	4.3
2	A	424	ALA	4.3
2	A	578	ALA	4.0
2	A	667	VAL	4.0
2	A	650	PHE	3.9
2	A	626	LYS	3.9
2	A	661	ASP	3.8
2	A	716	PHE	3.8
2	A	623	TRP	3.7
2	A	194	SER	3.6
2	A	376	ALA	3.6
2	A	662	ALA	3.6
2	A	630	GLY	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	A	659	ILE	3.6
2	A	656	GLY	3.5
2	A	428	ALA	3.5
2	A	688	ARG	3.4
2	A	598	LEU	3.4
2	A	373	GLY	3.4
2	A	583	GLY	3.3
2	A	621	PHE	3.3
2	A	657	TYR	3.3
2	A	644	GLN	3.2
2	A	671	VAL	3.2
2	A	703	ALA	3.2
2	A	660	MET	3.2
2	A	607	LEU	3.1
2	A	596	ALA	3.1
2	A	426	CYS	3.0
2	A	637	VAL	3.0
2	A	654	ILE	3.0
2	A	666	LEU	3.0
2	A	706	LEU	3.0
2	A	606	PHE	3.0
2	A	599	SER	2.9
2	A	375	VAL	2.9
2	A	642	LYS	2.9
2	A	577	LEU	2.9
2	A	651	ALA	2.9
2	A	579	LEU	2.9
2	A	628	ILE	2.8
2	A	535	PRO	2.8
2	A	597	ILE	2.7
2	A	674	TYR	2.7
2	A	712	CYS	2.7
2	A	584	TYR	2.7
2	A	527	THR	2.7
2	A	427	ASP	2.6
2	A	640	TYR	2.6
2	A	539	TYR	2.6
2	A	631	SER	2.5
2	A	647	ASN	2.4
2	A	184	ASP	2.3
2	A	421	GLY	2.3
2	A	670	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	705	TYR	2.3
2	A	634	ILE	2.2
2	A	645	LEU	2.2
2	A	197	ARG	2.2
2	A	611	SER	2.2
2	A	588	PHE	2.2
2	A	401	ASN	2.1
2	A	196	THR	2.1
2	A	378	LEU	2.1
2	A	518	ARG	2.1
2	A	686	TYR	2.1
2	A	257	ASN	2.1
2	A	652	GLU	2.1
2	A	399	SER	2.1
2	A	664	ASN	2.1
2	A	714	THR	2.1
2	A	675	PRO	2.1
2	A	633	GLN	2.0
2	A	682	ALA	2.0
2	A	618	GLY	2.0
2	A	663	THR	2.0
2	A	704	PRO	2.0
2	A	672	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.