Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:02 PM GMT

PDB ID	:	4E68
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)

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 (i)

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.
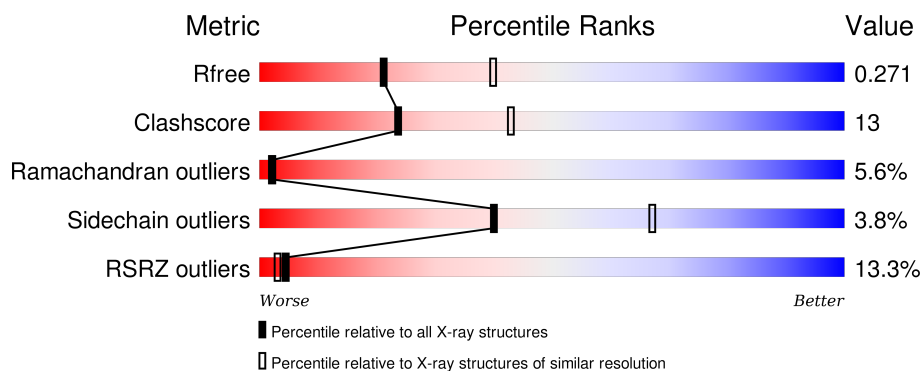
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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 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 <=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	61% 33% 6%
2	A	596	13% 66% 22% 5% 6%

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
1	B	18	Total	C	N	O	P	0	0	0
			360	175	59	109	17			

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

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

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	O	0	0
			24	24		
3	A	115	Total	O	0	0
			115	115		

3 Residue-property plots (i)

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.
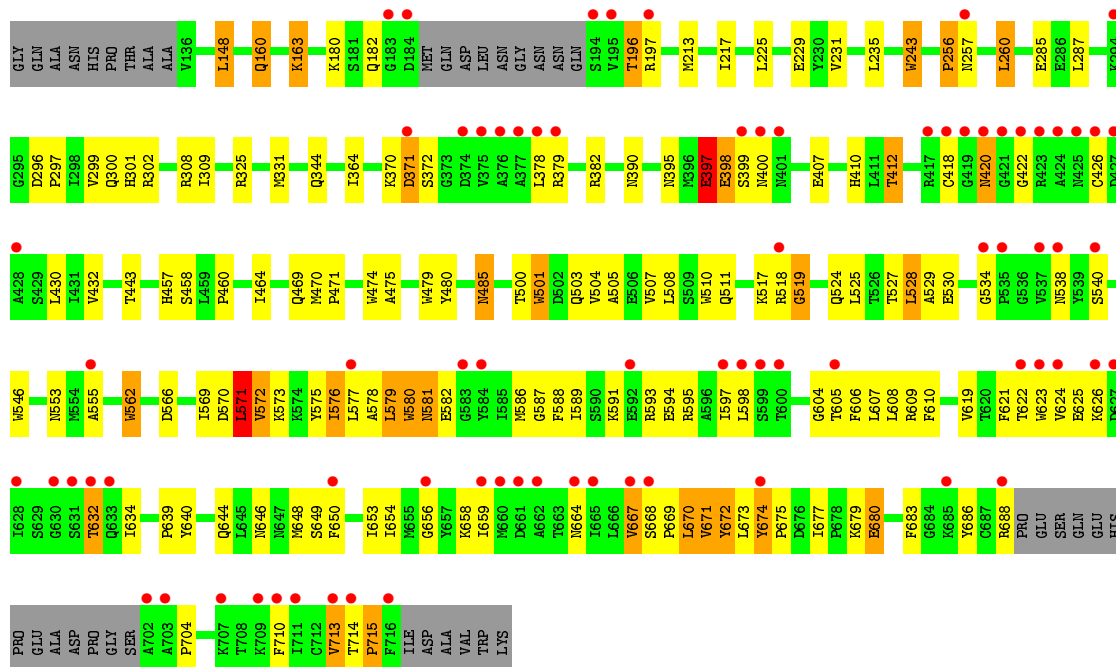
• Molecule 1: DNA (5'-D(*TP*GP*CP*AP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP*CP*T)-3')
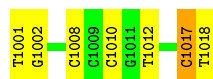
• Molecule 2: Signal transducer and activator of transcription 3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	174.14Å 174.14Å 79.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.58 14.98 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.1 (14.98-2.58) 97.6 (14.98-2.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.58Å)	Xtriage
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 (5.26%)	DCC
Wilson B-factor (Å^2)	60.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.3	EDS
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 36227 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/401	1.06	4/616 (0.6%)
2	A	0.60	8/4586 (0.2%)	0.83	3/6194 (0.0%)
All	All	0.58	8/4987 (0.2%)	0.85	7/6810 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	510	TRP	CD2-CE2	5.75	1.48	1.41
2	A	580	TRP	CD2-CE2	5.47	1.48	1.41
2	A	562	TRP	CD2-CE2	5.39	1.47	1.41
2	A	479	TRP	CD2-CE2	5.28	1.47	1.41
2	A	546	TRP	CD2-CE2	5.20	1.47	1.41
2	A	243	TRP	CD2-CE2	5.18	1.47	1.41
2	A	501	TRP	CD2-CE2	5.16	1.47	1.41
2	A	474	TRP	CD2-CE2	5.05	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1012	DT	P-O3'-C3'	8.16	129.49	119.70
2	A	528	LEU	CA-CB-CG	6.76	130.85	115.30
2	A	390	ASN	N-CA-CB	-6.62	98.69	110.60
1	B	1017	DC	P-O3'-C3'	6.41	127.40	119.70
1	B	1008	DC	P-O3'-C3'	6.40	127.38	119.70
2	A	571	LEU	CA-CB-CG	6.19	129.54	115.30
1	B	1010	DC	P-O3'-C3'	5.50	126.30	119.70

There are no chirality outliers.

There are no planarity outliers.

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	B	360	0	207	2	0
2	A	4499	0	4554	125	0
3	A	115	0	0	7	0
3	B	24	0	0	0	0
All	All	4998	0	4761	127	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 13.

All (127) 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:597:ILE:HG13	2:A:598:LEU:N	1.90	0.84
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: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:518:ARG:HG2	2:A:519:GLY:N	2.09	0.68
2:A:640:TYR:HB3	2:A:644:GLN:HB2	1.76	0.67
2:A:569:ILE:O	2:A:572:VAL:HG12	1.95	0.67
2:A:668:SER:HB2	2:A:669:PRO:HD2	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:597:ILE:CD1	2:A:622:THR:HG21	2.29	0.61
2:A:572:VAL:O	2:A:572:VAL:HG13	2.00	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: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: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:658:LYS:HA	2:A:668:SER:HA	1.91	0.53
2:A:527:THR:OG1	2:A:588:PHE:O	2.24	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:N	2:A:659:ILE:HD12	2.25	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:658:LYS:C	2:A:659:ILE:HD12	2.32	0.50
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
2:A:622:THR:HG23	2:A:634:ILE:HG23	1.94	0.49
2:A:160:GLN:NE2	2:A:160:GLN:HA	2.27	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:619:VAL:O	3:A:824:HOH:O	2.20	0.49
2:A:460:PRO:HG2	2:A:480:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:649:SER:O	2:A:653:ILE:HG13	2.12	0.49
2:A:679:LYS:HG3	2:A:679:LYS:O	2.12	0.49
2:A:639:PRO:HA	3:A:824:HOH:O	2.12	0.48
2:A:591:LYS:HA	2:A:594:GLU:HB3	1.96	0.48
2:A:300:GLN:HG3	2:A:301:HIS:CD2	2.49	0.48
2:A:648:MET:HE1	2:A:710:PHE:O	2.14	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:CD1	2:A:579:LEU:H	2.27	0.47
2:A:180:LYS:C	2:A:182:GLN:H	2.18	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:679:LYS:O	2:A:680:GLU:CB	2.64	0.46
2:A:213:MET:O	2:A:217:ILE:HG13	2.15	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:579:LEU:N	2:A:579:LEU:HD12	2.32	0.45
2:A:571:LEU:C	2:A:573:LYS:H	2.19	0.45
2:A:464:ILE:HB	2:A:469:GLN:OE1	2.17	0.45
2:A:507:VAL:O	2:A:511:GLN:HG2	2.16	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:N	2:A:485:ASN:HD22	2.09	0.44
2:A:325:ARG:NH2	2:A:407:GLU:OE2	2.51	0.44
2:A:581:ASN:ND2	2:A:686:TYR:OH	2.51	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:382:ARG:NH1	2:A:432:VAL:CG2	2.81	0.43
2:A:610:PHE:CD1	2:A:619:VAL:HG12	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:517:LYS:NZ	2:A:581:ASN:HA	2.34	0.43
2:A:673:LEU:N	2:A:677:ILE:O	2.49	0.43
2:A:517:LYS:NZ	2:A:577:LEU:O	2.50	0.42
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:HA	2:A:309:ILE:HD12	1.93	0.42
2:A:572:VAL:HG22	2:A:580:TRP:HB2	2.02	0.42
2:A:517:LYS:HZ2	2:A:581:ASN:CA	2.33	0.42
2:A:671:VAL:HA	2:A:679:LYS:HG2	2.02	0.41
2:A:589:ILE:HD11	2:A:593:ARG:HG3	2.02	0.41
2:A:670:LEU:N	2:A:670:LEU:HD22	2.35	0.41
2:A:517:LYS:HZ2	2:A:581:ASN:HA	1.85	0.41
2:A:650:PHE:HA	2:A:653:ILE:HD12	2.02	0.41
2:A:606:PHE:O	2:A:674:TYR:N	2.46	0.41
2:A:562:TRP:CE2	2:A:566:ASP:HB2	2.55	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:579:LEU:HD12	2:A:579:LEU:H	1.86	0.41
2:A:517:LYS:CE	2:A:581:ASN:HA	2.50	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%)	2 2

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%)	485 (96%)	19 (4%)	40 67

All (19) 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	287	LEU
2	A	331	MET
2	A	379	ARG
2	A	397	GLU
2	A	398	GLU
2	A	412	THR
2	A	420	ASN
2	A	485	ASN
2	A	579	LEU
2	A	670	LEU
2	A	671	VAL
2	A	688	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
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
2	A	457	HIS
2	A	472	ASN
2	A	485	ASN
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 carbohydrates 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 (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, 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	B	18/18 (100%)	-0.53	0	100	100	38, 50, 70, 82	0
2	A	559/596 (93%)	0.56	77 (13%)	4	2	33, 62, 142, 172	0
All	All	577/614 (93%)	0.52	77 (13%)	4	3	33, 61, 140, 172	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	426	CYS	13.6
2	A	702	ALA	10.1
2	A	622	THR	9.1
2	A	421	GLY	8.4
2	A	703	ALA	7.2
2	A	668	SER	6.5
2	A	633	GLN	6.4
2	A	420	ASN	6.4
2	A	195	VAL	6.2
2	A	184	ASP	6.1
2	A	632	THR	6.0
2	A	425	ASN	5.7
2	A	418	CYS	5.6
2	A	631	SER	5.3
2	A	377	ALA	4.9
2	A	376	ALA	4.8
2	A	659	ILE	4.7
2	A	401	ASN	4.7
2	A	194	SER	4.6
2	A	599	SER	4.6
2	A	627	ASP	4.4
2	A	623	TRP	4.4
2	A	688	ARG	4.3
2	A	626	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
2	A	422	GLY	4.2
2	A	656	GLY	4.2
2	A	375	VAL	4.1
2	A	600	THR	4.0
2	A	428	ALA	3.9
2	A	665	ILE	3.9
2	A	628	ILE	3.8
2	A	661	ASP	3.7
2	A	630	GLY	3.7
2	A	424	ALA	3.6
2	A	183	GLY	3.6
2	A	662	ALA	3.5
2	A	667	VAL	3.4
2	A	374	ASP	3.3
2	A	427	ASP	3.3
2	A	537	VAL	3.3
2	A	535	PRO	3.2
2	A	419	GLY	3.1
2	A	598	LEU	3.1
2	A	597	ILE	3.0
2	A	423	ARG	3.0
2	A	624	VAL	2.9
2	A	707	LYS	2.9
2	A	540	SER	2.8
2	A	555	ALA	2.8
2	A	534	GLY	2.8
2	A	417	ARG	2.8
2	A	711	ILE	2.8
2	A	710	PHE	2.7
2	A	605	THR	2.7
2	A	400	ASN	2.7
2	A	538	ASN	2.6
2	A	592	GLU	2.6
2	A	583	GLY	2.6
2	A	664	ASN	2.5
2	A	294	LYS	2.5
2	A	378	LEU	2.4
2	A	685	LYS	2.4
2	A	518	ARG	2.4
2	A	709	LYS	2.3
2	A	650	PHE	2.3
2	A	257	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	660	MET	2.2
2	A	716	PHE	2.2
2	A	371	ASP	2.2
2	A	399	SER	2.2
2	A	584	TYR	2.2
2	A	674	TYR	2.2
2	A	713	VAL	2.1
2	A	197	ARG	2.1
2	A	714	THR	2.0
2	A	379	ARG	2.0
2	A	577	LEU	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.