Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:43 AM GMT

PDB ID	:	3BXJ
Title	:	Crystal Structure of the C2-GAP Fragment of synGAP
Authors	:	Pena, V.; Hothorn, M.; Eberth, A.; Kaschau, N.; Parret, A.; Gremer, L.; Bonneau, F.; Ahmadian, M.R.; Scheffzek, K.
Deposited on	:	2008-01-14
Resolution	:	3.00 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 ①) were used in the production of this report:

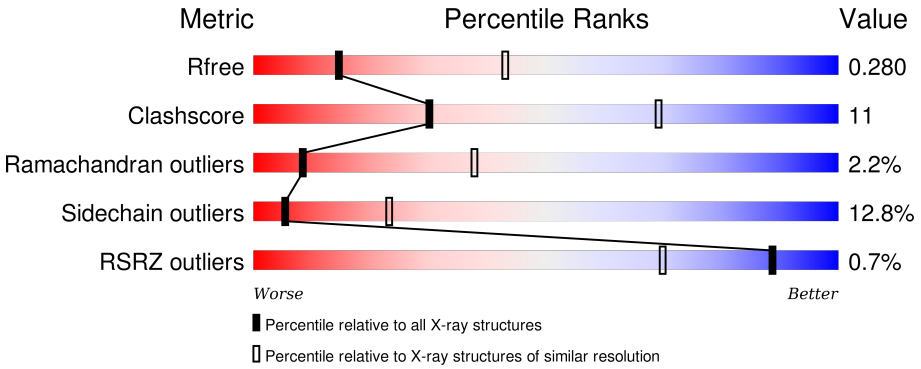
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	A	483	54% 14% • 28%
1	B	483	% 54% 16% • 26%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5491 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 Ras GTPase-activating protein SynGAP.

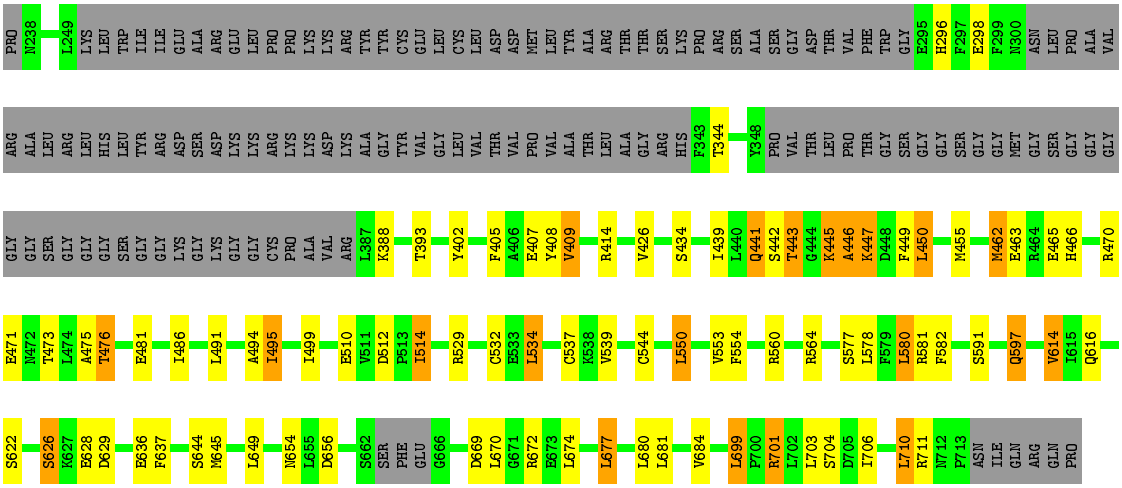
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2695	1711	458	505	21			
1	B	358	Total	C	N	O	S	0	0	0
			2796	1774	474	527	21			

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.

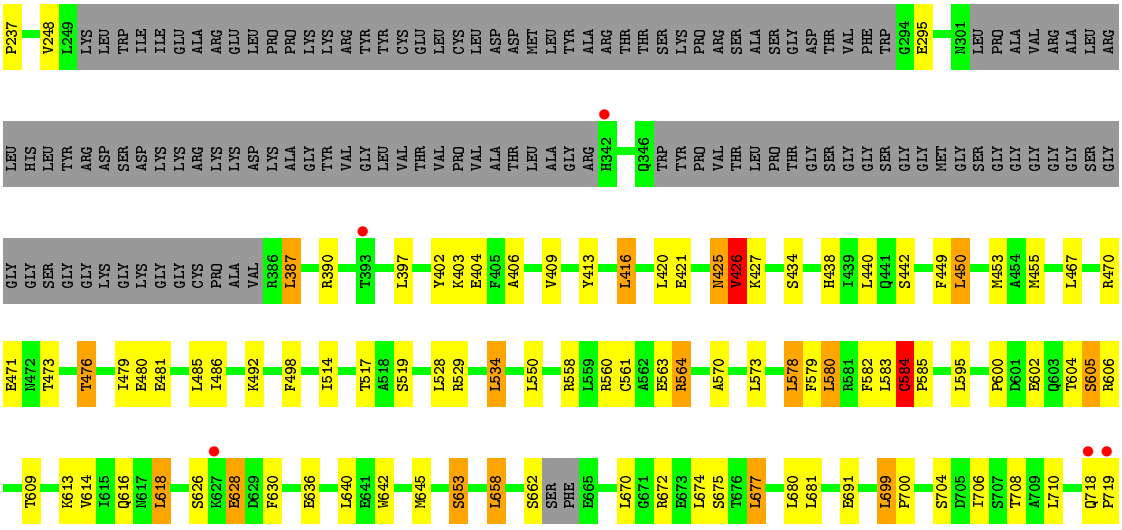
- Molecule 1: Ras GTPase-activating protein SynGAP

Chain A:



- Molecule 1: Ras GTPase-activating protein SynGAP

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	113.32Å 113.32Å 166.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.00 19.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-3.00) 99.5 (19.80-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.289 0.233 , 0.280	Depositor DCC
R_{free} test set	1206 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.7	EDS
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 32876 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5491	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.72	1/2738 (0.0%)	0.74	0/3693
1	B	0.76	1/2842 (0.0%)	0.80	2/3832 (0.1%)
All	All	0.74	2/5580 (0.0%)	0.77	2/7525 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	GLU	CB-CG	5.81	1.63	1.52
1	A	537	CYS	CB-SG	-5.81	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	719	PRO	N-CA-CB	6.42	111.01	103.30
1	B	237	PRO	N-CA-CB	5.92	110.41	103.30

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	2695	0	2604	67	0
1	B	2796	0	2714	56	0
All	All	5491	0	5318	120	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 11.

All (120) 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:B:470:ARG:O	1:B:476:THR:HG21	1.62	1.00
1:A:470:ARG:O	1:A:476:THR:HG21	1.65	0.95
1:A:462:MET:HE2	1:A:462:MET:HA	1.57	0.85
1:A:462:MET:CE	1:A:462:MET:HA	2.10	0.82
1:B:563:GLU:O	1:B:564:ARG:HB2	1.81	0.80
1:A:580:LEU:HA	1:A:616:GLN:NE2	1.98	0.78
1:A:486:ILE:HD11	1:A:550:LEU:HD12	1.63	0.77
1:B:605:SER:O	1:B:609:THR:HG23	1.83	0.76
1:A:473:THR:HB	1:A:476:THR:HG23	1.69	0.73
1:A:580:LEU:CA	1:A:616:GLN:HE22	2.01	0.72
1:A:408:TYR:O	1:A:409:VAL:HB	1.89	0.72
1:A:445:LYS:O	1:A:446:ALA:HB3	1.90	0.71
1:B:397:LEU:HD11	1:B:706:ILE:HG23	1.73	0.70
1:B:498:PHE:CD1	1:B:534:LEU:HD13	2.27	0.70
1:B:517:THR:HG22	1:B:519:SER:H	1.57	0.70
1:B:425:ASN:HD22	1:B:426:VAL:HG23	1.57	0.69
1:B:613:LYS:HD3	1:B:628:GLU:OE1	1.94	0.68
1:A:580:LEU:HA	1:A:616:GLN:HE22	1.55	0.68
1:B:582:PHE:O	1:B:583:LEU:HB3	1.94	0.65
1:B:579:PHE:O	1:B:584:CYS:HB2	1.97	0.65
1:B:473:THR:HG22	1:B:476:THR:H	1.62	0.65
1:A:408:TYR:O	1:A:409:VAL:CB	2.45	0.63
1:B:473:THR:HB	1:B:476:THR:HG23	1.81	0.61
1:A:405:PHE:O	1:A:408:TYR:O	2.17	0.61
1:A:470:ARG:O	1:A:476:THR:CG2	2.43	0.61
1:A:512:ASP:OD2	1:A:514:ILE:HG12	2.01	0.60
1:A:445:LYS:O	1:A:446:ALA:CB	2.50	0.60
1:B:704:SER:O	1:B:708:THR:HG23	2.02	0.60
1:A:441:GLN:HE21	1:A:441:GLN:CA	2.16	0.59
1:B:486:ILE:C	1:B:486:ILE:HD12	2.25	0.57
1:B:584:CYS:CB	1:B:585:PRO:HD3	2.35	0.57
1:A:491:LEU:HD22	1:A:582:PHE:CZ	2.39	0.57
1:A:706:ILE:HG22	1:A:710:LEU:HD12	1.87	0.57
1:A:677:LEU:HD22	1:A:681:LEU:CD1	2.35	0.56
1:A:473:THR:CG2	1:A:475:ALA:HB3	2.35	0.56
1:A:441:GLN:HE21	1:A:441:GLN:HA	1.70	0.56
1:A:473:THR:HG22	1:A:475:ALA:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:CYS:HB3	1:B:585:PRO:HD3	1.87	0.56
1:A:645:MET:HE2	1:A:645:MET:O	2.07	0.55
1:A:486:ILE:HD11	1:A:550:LEU:CD1	2.33	0.55
1:B:425:ASN:O	1:B:427:LYS:N	2.40	0.54
1:B:580:LEU:HA	1:B:616:GLN:HE22	1.73	0.54
1:B:449:PHE:O	1:B:450:LEU:HG	2.06	0.54
1:A:473:THR:HG22	1:A:475:ALA:N	2.22	0.54
1:B:409:VAL:HG12	1:B:440:LEU:HD21	1.90	0.54
1:A:439:ILE:CD1	1:A:677:LEU:HD12	2.38	0.54
1:B:434:SER:O	1:B:438:HIS:HD2	1.92	0.53
1:A:446:ALA:O	1:A:447:LYS:HB2	2.08	0.53
1:A:701:ARG:HA	1:A:704:SER:OG	2.08	0.53
1:A:534:LEU:HD22	1:A:534:LEU:O	2.08	0.53
1:B:248:VAL:HA	1:B:387:LEU:HD22	1.90	0.53
1:A:532:CYS:SG	1:A:614:VAL:HG21	2.49	0.52
1:B:558:ARG:HD2	1:B:653:SER:OG	2.10	0.52
1:B:434:SER:HA	1:B:481:GLU:HG2	1.91	0.52
1:B:600:PRO:HB3	1:B:604:THR:HB	1.93	0.51
1:A:677:LEU:HD22	1:A:681:LEU:HD11	1.92	0.51
1:A:449:PHE:O	1:A:450:LEU:HB2	2.11	0.51
1:A:597:GLN:HE21	1:A:597:GLN:HA	1.75	0.51
1:B:498:PHE:HD1	1:B:534:LEU:HD13	1.74	0.50
1:A:699:LEU:HD13	1:A:703:LEU:HD11	1.92	0.50
1:A:443:THR:O	1:A:443:THR:HG23	2.10	0.50
1:B:677:LEU:HD22	1:B:681:LEU:HG	1.94	0.49
1:A:669:ASP:OD2	1:A:672:ARG:HB2	2.11	0.49
1:A:441:GLN:NE2	1:A:441:GLN:HA	2.28	0.49
1:A:495:ILE:HG23	1:A:499:ILE:HG13	1.94	0.49
1:B:449:PHE:O	1:B:450:LEU:CB	2.61	0.48
1:B:397:LEU:CD1	1:B:706:ILE:HG23	2.40	0.48
1:B:578:LEU:O	1:B:582:PHE:O	2.31	0.48
1:A:495:ILE:HD11	1:A:539:VAL:CG2	2.43	0.48
1:A:455:MET:HG3	1:A:560:ARG:HD2	1.95	0.48
1:B:618:LEU:HB3	1:B:645:MET:HE2	1.94	0.48
1:A:486:ILE:O	1:A:486:ILE:HD12	2.14	0.48
1:B:582:PHE:O	1:B:583:LEU:CB	2.61	0.48
1:B:402:TYR:HB3	1:B:674:LEU:HD13	1.96	0.47
1:A:471:GLU:O	1:A:473:THR:N	2.47	0.47
1:B:455:MET:HE1	1:B:573:LEU:HD12	1.96	0.47
1:B:584:CYS:CB	1:B:585:PRO:CD	2.93	0.47
1:B:416:LEU:HD22	1:B:420:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LEU:N	1:A:616:GLN:HE22	2.13	0.46
1:B:640:LEU:HD23	1:B:640:LEU:O	2.14	0.46
1:A:473:THR:HG21	1:A:475:ALA:HB3	1.97	0.46
1:A:495:ILE:HD11	1:A:539:VAL:HG23	1.98	0.46
1:A:439:ILE:HD13	1:A:677:LEU:HD12	1.98	0.45
1:A:449:PHE:O	1:A:450:LEU:CB	2.65	0.45
1:A:446:ALA:O	1:A:447:LYS:CB	2.65	0.45
1:B:580:LEU:HA	1:B:616:GLN:NE2	2.31	0.45
1:A:514:ILE:H	1:A:514:ILE:HD13	1.82	0.45
1:B:699:LEU:N	1:B:700:PRO:HD2	2.32	0.45
1:A:441:GLN:HE21	1:A:441:GLN:C	2.20	0.45
1:B:561:CYS:SG	1:B:570:ALA:HB2	2.57	0.44
1:B:476:THR:HA	1:B:479:ILE:HD12	1.99	0.44
1:A:471:GLU:HG2	1:A:581:ARG:HH21	1.82	0.44
1:A:486:ILE:HD11	1:A:550:LEU:CG	2.47	0.44
1:B:467:LEU:O	1:B:470:ARG:HD3	2.18	0.44
1:A:471:GLU:HG3	1:B:560:ARG:CD	2.47	0.44
1:A:645:MET:HE2	1:A:649:LEU:HG	1.99	0.44
1:B:492:LYS:HG2	1:B:595:LEU:HD23	1.99	0.44
1:B:449:PHE:O	1:B:450:LEU:CG	2.66	0.44
1:A:473:THR:HG22	1:A:475:ALA:HB3	1.99	0.43
1:B:613:LYS:CD	1:B:628:GLU:OE1	2.65	0.43
1:B:403:LYS:O	1:B:406:ALA:HB3	2.19	0.43
1:B:514:ILE:O	1:B:514:ILE:HG22	2.18	0.43
1:A:471:GLU:HG3	1:B:560:ARG:HD2	1.99	0.43
1:B:602:GLU:CD	1:B:602:GLU:H	2.22	0.43
1:A:344:THR:CB	1:A:388:LYS:HE3	2.49	0.43
1:B:580:LEU:CA	1:B:616:GLN:HE22	2.31	0.42
1:B:471:GLU:OE2	1:B:480:GLU:OE2	2.37	0.42
1:A:441:GLN:NE2	1:A:441:GLN:CA	2.79	0.42
1:A:402:TYR:HB3	1:A:674:LEU:HD13	2.02	0.42
1:B:434:SER:O	1:B:438:HIS:CD2	2.72	0.42
1:A:550:LEU:HD22	1:A:554:PHE:CZ	2.54	0.42
1:A:442:SER:OG	1:A:670:LEU:HD22	2.21	0.41
1:A:447:LYS:HA	1:A:553:VAL:HG22	2.03	0.41
1:A:434:SER:HA	1:A:481:GLU:HG3	2.03	0.41
1:B:449:PHE:O	1:B:449:PHE:CD2	2.73	0.41
1:B:413:TYR:CE1	1:B:449:PHE:HB2	2.56	0.41
1:A:560:ARG:O	1:A:564:ARG:HG2	2.21	0.41
1:A:680:LEU:CD2	1:B:658:LEU:HD21	2.51	0.41
1:A:529:ARG:NH1	1:A:637:PHE:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:O	1:A:684:VAL:HG23	2.22	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	338/483 (70%)	308 (91%)	22 (6%)	8 (2%)	7	35
1	B	348/483 (72%)	318 (91%)	23 (7%)	7 (2%)	9	41
All	All	686/966 (71%)	626 (91%)	45 (7%)	15 (2%)	8	38

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	VAL
1	A	447	LYS
1	A	494	ALA
1	B	295	GLU
1	B	450	LEU
1	B	453	MET
1	B	584	CYS
1	B	718	GLN
1	A	450	LEU
1	B	426	VAL
1	A	296	HIS
1	A	466	HIS
1	A	626	SER
1	B	564	ARG
1	A	446	ALA

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	278/413 (67%)	241 (87%)	37 (13%)	5 21
1	B	294/413 (71%)	258 (88%)	36 (12%)	6 25
All	All	572/826 (69%)	499 (87%)	73 (13%)	5 23

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	393	THR
1	A	407	GLU
1	A	414	ARG
1	A	426	VAL
1	A	441	GLN
1	A	443	THR
1	A	445	LYS
1	A	462	MET
1	A	463	GLU
1	A	465	GLU
1	A	476	THR
1	A	495	ILE
1	A	510	GLU
1	A	514	ILE
1	A	534	LEU
1	A	544	CYS
1	A	550	LEU
1	A	577	SER
1	A	578	LEU
1	A	580	LEU
1	A	591	SER
1	A	597	GLN
1	A	614	VAL
1	A	622	SER
1	A	626	SER
1	A	628	GLU

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Mol	Chain	Res	Type
1	A	629	ASP
1	A	636	GLU
1	A	644	SER
1	A	654	ASN
1	A	656	ASP
1	A	677	LEU
1	A	699	LEU
1	A	701	ARG
1	A	710	LEU
1	A	711	ARG
1	B	387	LEU
1	B	390	ARG
1	B	416	LEU
1	B	421	GLU
1	B	425	ASN
1	B	426	VAL
1	B	442	SER
1	B	476	THR
1	B	485	LEU
1	B	528	LEU
1	B	529	ARG
1	B	534	LEU
1	B	550	LEU
1	B	578	LEU
1	B	580	LEU
1	B	584	CYS
1	B	605	SER
1	B	606	ARG
1	B	614	VAL
1	B	618	LEU
1	B	626	SER
1	B	628	GLU
1	B	630	PHE
1	B	636	GLU
1	B	642	TRP
1	B	653	SER
1	B	658	LEU
1	B	662	SER
1	B	670	LEU
1	B	672	ARG
1	B	675	SER
1	B	677	LEU

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Mol	Chain	Res	Type
1	B	680	LEU
1	B	691	GLU
1	B	699	LEU
1	B	710	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	ASN
1	A	597	GLN
1	A	616	GLN
1	B	425	ASN
1	B	438	HIS
1	B	441	GLN
1	B	472	ASN
1	B	541	ASN
1	B	616	GLN
1	B	646	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} 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	348/483 (72%)	-0.56	0 100 100	35, 46, 60, 66	0
1	B	358/483 (74%)	-0.50	5 (1%) 78 51	36, 46, 55, 65	0
All	All	706/966 (73%)	-0.53	5 (0%) 89 70	35, 46, 58, 66	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	718	GLN	3.6
1	B	342	HIS	2.6
1	B	719	PRO	2.2
1	B	627	LYS	2.2
1	B	393	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.