Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:14 AM GMT

PDB ID	:	2PZ1
Title	:	Crystal Structure of Auto-inhibited Asef
Authors	:	Betts, L.; Sondek, J.; Rossman, K.L.
Deposited on	:	2007-05-17
Resolution	:	2.25 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

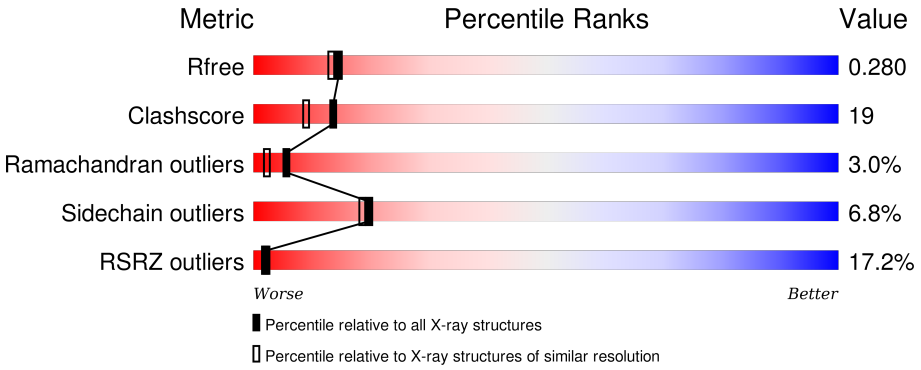
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	466	15% 61% 22% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3430 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 Rho guanine nucleotide exchange factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3330	2091	601	619	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	GLY	-	CLONING ARTIFACT	UNP Q9NR80
A	168	ALA	-	CLONING ARTIFACT	UNP Q9NR80
A	169	MET	-	CLONING ARTIFACT	UNP Q9NR80

- Molecule 2 is water.

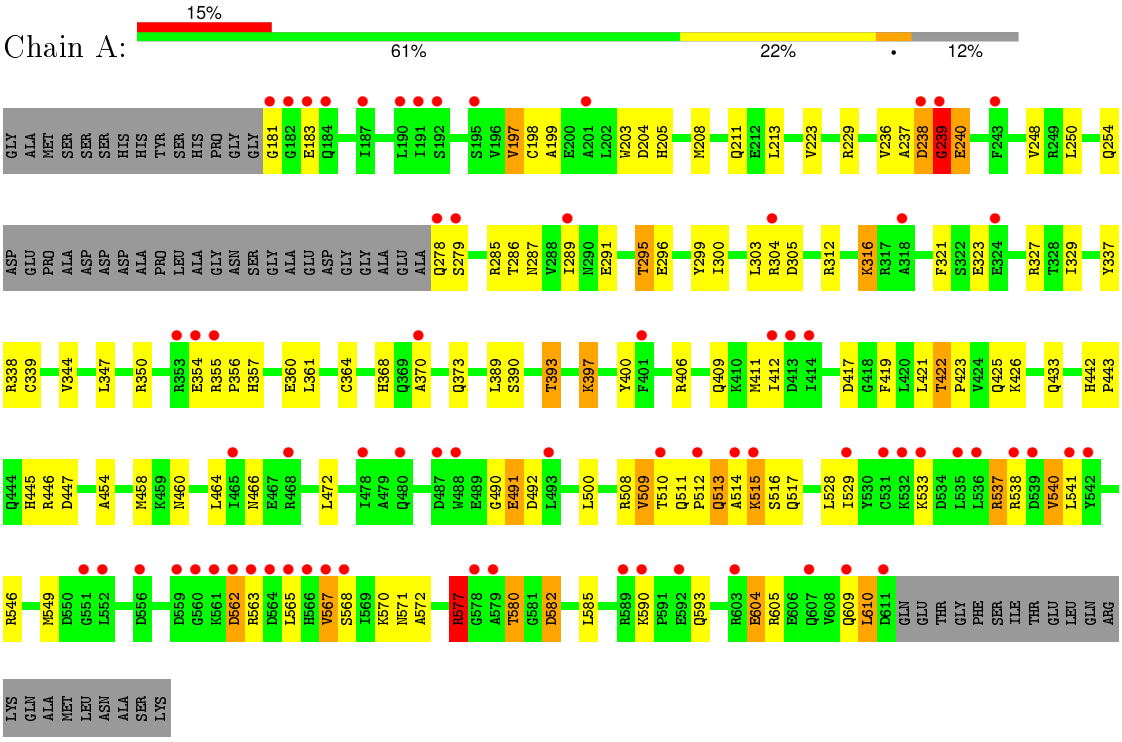
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		

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: Rho guanine nucleotide exchange factor 4

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.42Å 79.88Å 67.41Å 90.00° 122.99° 90.00°	Depositor
Resolution (Å)	15.00 – 2.25 14.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.25) 98.9 (14.88-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.279 0.216 , 0.280	Depositor DCC
R_{free} test set	1071 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 20925 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3430	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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	0.32	0/3394	0.51	1/4565 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	GLY	N-CA-C	-7.20	95.11	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	GLY	Peptide

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	3330	0	3238	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	100	0	0	8	0
All	All	3430	0	3238	122	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 19.

All (122) 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:304:ARG:HH11	1:A:304:ARG:HG2	1.20	1.06
1:A:513:GLN:HG2	1:A:514:ALA:HB2	1.36	1.05
1:A:513:GLN:CG	1:A:514:ALA:HB2	1.90	1.01
1:A:198:CYS:SG	2:A:82:HOH:O	2.18	1.01
1:A:577:ARG:HH11	1:A:577:ARG:CG	1.80	0.93
1:A:528:LEU:HB2	1:A:549:MET:CE	1.97	0.93
1:A:577:ARG:HH11	1:A:577:ARG:HG2	1.32	0.92
1:A:512:PRO:O	1:A:513:GLN:HB2	1.65	0.91
1:A:198:CYS:H	1:A:254:GLN:HE22	1.17	0.88
1:A:513:GLN:HG2	1:A:514:ALA:CB	2.04	0.88
1:A:490:GLY:O	1:A:491:GLU:CB	2.21	0.87
1:A:528:LEU:HB2	1:A:549:MET:HE2	1.56	0.86
1:A:609:GLN:HG3	1:A:610:LEU:N	1.92	0.84
1:A:445:HIS:HD2	1:A:447:ASP:H	1.28	0.82
1:A:537:ARG:HB3	1:A:540:VAL:CG1	2.08	0.82
1:A:577:ARG:HG2	1:A:577:ARG:NH1	1.92	0.78
1:A:213:LEU:HD13	1:A:240:GLU:H	1.49	0.78
1:A:490:GLY:O	1:A:491:GLU:HB3	1.84	0.77
1:A:295:THR:HG21	1:A:433:GLN:HE22	1.49	0.77
1:A:528:LEU:CB	1:A:549:MET:HE2	2.15	0.76
1:A:528:LEU:CB	1:A:549:MET:CE	2.64	0.75
1:A:312:ARG:O	1:A:316:LYS:HD2	1.86	0.75
1:A:304:ARG:NH1	1:A:305:ASP:OD1	2.19	0.75
1:A:609:GLN:HG3	1:A:610:LEU:H	1.51	0.75
1:A:580:THR:OG1	1:A:582:ASP:OD1	2.03	0.74
1:A:421:LEU:HD23	2:A:92:HOH:O	1.86	0.74
1:A:304:ARG:HG2	1:A:304:ARG:NH1	1.99	0.72
1:A:181:GLY:N	2:A:8:HOH:O	2.22	0.71
1:A:513:GLN:HA	1:A:514:ALA:HB2	1.74	0.69
1:A:239:GLY:HA2	1:A:240:GLU:HB2	1.75	0.69
1:A:528:LEU:HB2	1:A:549:MET:HE3	1.77	0.67
1:A:239:GLY:CA	1:A:240:GLU:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:PHE:O	1:A:422:THR:HB	1.97	0.65
1:A:205:HIS:HD2	1:A:213:LEU:O	1.80	0.64
1:A:490:GLY:O	1:A:491:GLU:HB2	1.97	0.64
1:A:406:ARG:HA	1:A:411:MET:CE	2.28	0.63
1:A:370:ALA:HA	1:A:373:GLN:HG2	1.82	0.61
1:A:312:ARG:O	1:A:316:LYS:CD	2.48	0.60
1:A:329:ILE:HG23	1:A:389:LEU:HD21	1.83	0.60
1:A:397:LYS:HE2	2:A:96:HOH:O	2.01	0.59
1:A:537:ARG:HB3	1:A:540:VAL:HG12	1.86	0.58
1:A:570:LYS:O	1:A:572:ALA:N	2.37	0.58
1:A:511:GLN:O	1:A:512:PRO:C	2.42	0.57
1:A:537:ARG:HB3	1:A:540:VAL:HG13	1.83	0.57
1:A:515:LYS:HE2	1:A:516:SER:H	1.68	0.57
1:A:355:ARG:NH1	1:A:357:HIS:NE2	2.52	0.57
1:A:204:ASP:H	1:A:466:ASN:HD21	1.52	0.57
1:A:203:TRP:HA	1:A:466:ASN:ND2	2.20	0.57
1:A:513:GLN:CA	1:A:514:ALA:HB2	2.34	0.56
1:A:604:GLU:OE2	1:A:605:ARG:NE	2.27	0.56
1:A:364:CYS:O	1:A:368:HIS:HD2	1.89	0.56
1:A:422:THR:HG22	1:A:423:PRO:HD3	1.88	0.56
1:A:533:LYS:NZ	1:A:538:ARG:O	2.35	0.56
1:A:199:ALA:HB1	1:A:248:VAL:HG13	1.88	0.55
1:A:609:GLN:CG	1:A:610:LEU:N	2.69	0.55
1:A:237:ALA:O	1:A:238:ASP:CB	2.55	0.55
1:A:491:GLU:HG3	1:A:492:ASP:H	1.72	0.55
1:A:181:GLY:HA2	1:A:287:ASN:ND2	2.22	0.55
1:A:512:PRO:O	1:A:513:GLN:CB	2.48	0.54
1:A:291:GLU:O	1:A:295:THR:HB	2.06	0.54
1:A:213:LEU:HD13	1:A:240:GLU:N	2.21	0.53
1:A:285:ARG:NH1	1:A:289:ILE:HD11	2.24	0.53
1:A:350:ARG:HD3	1:A:360:GLU:O	2.09	0.53
1:A:577:ARG:CG	1:A:577:ARG:NH1	2.50	0.53
1:A:442:HIS:CG	1:A:443:PRO:HD2	2.45	0.52
1:A:406:ARG:HA	1:A:411:MET:HE3	1.90	0.52
1:A:237:ALA:O	1:A:238:ASP:HB2	2.09	0.51
1:A:529:ILE:HD13	1:A:546:ARG:HB2	1.92	0.51
1:A:213:LEU:CD1	1:A:240:GLU:H	2.20	0.51
1:A:299:TYR:CE1	1:A:422:THR:HG23	2.46	0.51
1:A:508:ARG:HH11	1:A:517:GLN:HE22	1.59	0.51
1:A:609:GLN:CG	1:A:610:LEU:H	2.21	0.50
1:A:442:HIS:CD2	1:A:443:PRO:HD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLU:HG3	1:A:492:ASP:N	2.27	0.50
1:A:537:ARG:CB	1:A:540:VAL:CG1	2.86	0.50
1:A:445:HIS:CD2	1:A:447:ASP:H	2.18	0.49
1:A:299:TYR:HE1	1:A:422:THR:HG23	1.77	0.49
1:A:181:GLY:HA2	1:A:287:ASN:HD21	1.75	0.49
1:A:203:TRP:CH2	1:A:425:GLN:HG2	2.48	0.49
1:A:197:VAL:CG2	1:A:223:VAL:HB	2.44	0.48
1:A:300:ILE:HG13	1:A:344:VAL:HG21	1.96	0.47
1:A:590:LYS:O	1:A:593:GLN:HB2	2.14	0.47
1:A:454:ALA:O	1:A:458:MET:HG2	2.15	0.47
1:A:511:GLN:H	1:A:512:PRO:HD2	1.80	0.47
1:A:562:ASP:H	1:A:567:VAL:CA	2.26	0.47
1:A:577:ARG:HH11	1:A:577:ARG:HG3	1.73	0.47
1:A:205:HIS:HE1	2:A:89:HOH:O	1.97	0.46
1:A:541:LEU:HD12	1:A:541:LEU:N	2.30	0.46
1:A:286:THR:HG23	1:A:356:PRO:HB2	1.98	0.46
1:A:312:ARG:HE	1:A:312:ARG:HB2	1.33	0.46
1:A:236:VAL:CG1	1:A:237:ALA:N	2.79	0.46
1:A:508:ARG:HH11	1:A:517:GLN:NE2	2.14	0.45
1:A:321:PHE:O	2:A:46:HOH:O	2.20	0.45
1:A:528:LEU:HB3	1:A:549:MET:HE2	1.98	0.45
1:A:510:THR:HG22	1:A:513:GLN:H	1.82	0.44
1:A:604:GLU:HG3	2:A:6:HOH:O	2.16	0.44
1:A:357:HIS:CD2	1:A:357:HIS:H	2.35	0.44
1:A:338:ARG:NH1	1:A:339:CYS:SG	2.91	0.44
1:A:515:LYS:HG3	1:A:516:SER:N	2.33	0.43
1:A:515:LYS:HG3	1:A:516:SER:H	1.84	0.43
1:A:406:ARG:HA	1:A:411:MET:HE2	1.98	0.43
1:A:390:SER:O	1:A:393:THR:HB	2.18	0.43
1:A:491:GLU:CG	1:A:492:ASP:H	2.32	0.43
1:A:537:ARG:CB	1:A:540:VAL:HG13	2.46	0.43
1:A:303:LEU:HD13	1:A:337:TYR:HA	2.01	0.43
1:A:208:MET:HG3	1:A:500:LEU:HD22	2.00	0.42
1:A:211:GLN:HA	1:A:211:GLN:NE2	2.34	0.42
1:A:513:GLN:HG3	1:A:514:ALA:HB2	1.90	0.42
1:A:577:ARG:NH1	2:A:78:HOH:O	2.53	0.42
1:A:199:ALA:HB2	1:A:250:LEU:HD23	2.01	0.42
1:A:509:VAL:HG13	1:A:585:LEU:HB3	2.02	0.42
1:A:412:ILE:H	1:A:412:ILE:HG12	1.57	0.42
1:A:400:TYR:N	1:A:400:TYR:CD2	2.87	0.42
1:A:357:HIS:O	1:A:445:HIS:HE1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:CG	1:A:304:ARG:NH1	2.69	0.41
1:A:355:ARG:HB3	1:A:357:HIS:NE2	2.35	0.41
1:A:296:GLU:HG3	1:A:347:LEU:HD23	2.02	0.41
1:A:562:ASP:N	1:A:567:VAL:O	2.54	0.41
1:A:323:GLU:HG3	1:A:327:ARG:HE	1.86	0.40
1:A:409:GLN:HB3	1:A:411:MET:CE	2.51	0.40
1:A:329:ILE:HG23	1:A:389:LEU:CD2	2.49	0.40
1:A:460:ASN:O	1:A:464:LEU:HD13	2.21	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	404/466 (87%)	372 (92%)	20 (5%)	12 (3%)	5 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ASP
1	A	240	GLU
1	A	491	GLU
1	A	513	GLN
1	A	562	ASP
1	A	563	ARG
1	A	565	LEU
1	A	577	ARG
1	A	571	ASN
1	A	580	THR
1	A	568	SER
1	A	567	VAL

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	354/405 (87%)	330 (93%)	24 (7%)	20 18

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	GLU
1	A	197	VAL
1	A	229	ARG
1	A	278	GLN
1	A	279	SER
1	A	295	THR
1	A	316	LYS
1	A	354	GLU
1	A	361	LEU
1	A	393	THR
1	A	397	LYS
1	A	417	ASP
1	A	422	THR
1	A	426	LYS
1	A	446	ARG
1	A	472	LEU
1	A	509	VAL
1	A	515	LYS
1	A	537	ARG
1	A	540	VAL
1	A	577	ARG
1	A	582	ASP
1	A	604	GLU
1	A	610	LEU

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

Mol	Chain	Res	Type
1	A	205	HIS

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	228	ASN
1	A	254	GLN
1	A	278	GLN
1	A	340	GLN
1	A	368	HIS
1	A	373	GLN
1	A	381	ASN
1	A	382	HIS
1	A	409	GLN
1	A	433	GLN
1	A	445	HIS
1	A	466	ASN
1	A	511	GLN
1	A	517	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	408/466 (87%)	0.96	70 (17%) 2 2	32, 51, 64, 84	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	GLY	7.1
1	A	184	GLN	6.9
1	A	564	ASP	5.4
1	A	278	GLN	5.1
1	A	568	SER	5.1
1	A	541	LEU	5.0
1	A	563	ARG	4.8
1	A	567	VAL	4.6
1	A	512	PRO	4.6
1	A	536	LEU	4.5
1	A	413	ASP	4.4
1	A	238	ASP	4.3
1	A	538	ARG	4.2
1	A	539	ASP	4.2
1	A	181	GLY	4.2
1	A	535	LEU	4.2
1	A	183	GLU	3.9
1	A	551	GLY	3.9
1	A	279	SER	3.7
1	A	559	ASP	3.6
1	A	562	ASP	3.6
1	A	611	ASP	3.6
1	A	353	ARG	3.6
1	A	565	LEU	3.5
1	A	531	CYS	3.5
1	A	603	ARG	3.5
1	A	566	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	578	GLY	3.3
1	A	487	ASP	3.3
1	A	191	ILE	3.3
1	A	370	ALA	3.1
1	A	579	ALA	3.1
1	A	609	GLN	3.0
1	A	190	LEU	3.0
1	A	542	TYR	2.9
1	A	552	LEU	2.9
1	A	355	ARG	2.9
1	A	529	ILE	2.9
1	A	239	GLY	2.9
1	A	201	ALA	2.8
1	A	515	LYS	2.8
1	A	493	LEU	2.7
1	A	243	PHE	2.7
1	A	289	ILE	2.6
1	A	465	ILE	2.6
1	A	590	LYS	2.5
1	A	556	ASP	2.4
1	A	589	ARG	2.4
1	A	607	GLN	2.4
1	A	192	SER	2.4
1	A	468	ARG	2.4
1	A	354	GLU	2.4
1	A	412	ILE	2.4
1	A	514	ALA	2.4
1	A	561	LYS	2.3
1	A	592	GLU	2.3
1	A	401	PHE	2.3
1	A	182	GLY	2.3
1	A	304	ARG	2.3
1	A	318	ALA	2.3
1	A	414	ILE	2.2
1	A	533	LYS	2.2
1	A	488	TRP	2.1
1	A	532	LYS	2.1
1	A	510	THR	2.1
1	A	187	ILE	2.1
1	A	324	GLU	2.1
1	A	478	ILE	2.1
1	A	480	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	195	SER	2.0

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.