Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:35 am BST

PDB ID	:	6D22
Title	:	Crystal structure of Tyrosine-protein kinase receptor
Authors	:	Greasley, S.E.; Brown, D.
Deposited on	:	2018-04-12
Resolution	:	2.46 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
https://www.wwpdb.org/validation/2017/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:

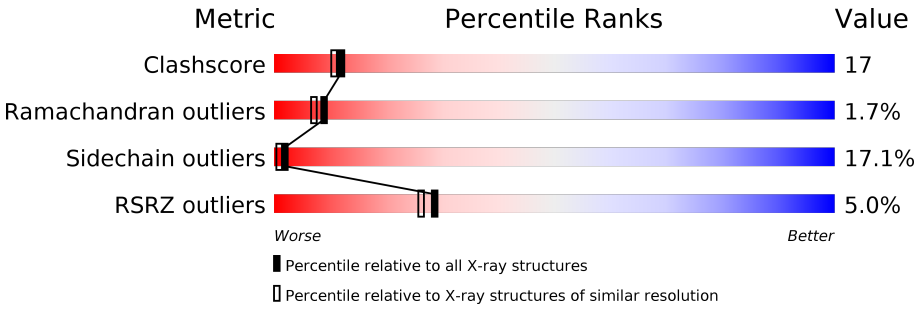
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.46 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))
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 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 <=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	307	5% 52% 33% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2553 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 Tyrosine-protein kinase receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2388	1526	430	417	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	490	HIS	-	expression tag	UNP J3KP20
A	491	HIS	-	expression tag	UNP J3KP20
A	492	HIS	-	expression tag	UNP J3KP20
A	493	HIS	-	expression tag	UNP J3KP20
A	494	HIS	-	expression tag	UNP J3KP20
A	495	HIS	-	expression tag	UNP J3KP20
A	496	LEU	-	expression tag	UNP J3KP20
A	497	VAL	-	expression tag	UNP J3KP20
A	498	PRO	-	expression tag	UNP J3KP20
A	499	ARG	-	expression tag	UNP J3KP20
A	500	GLY	-	expression tag	UNP J3KP20
A	501	SER	-	expression tag	UNP J3KP20

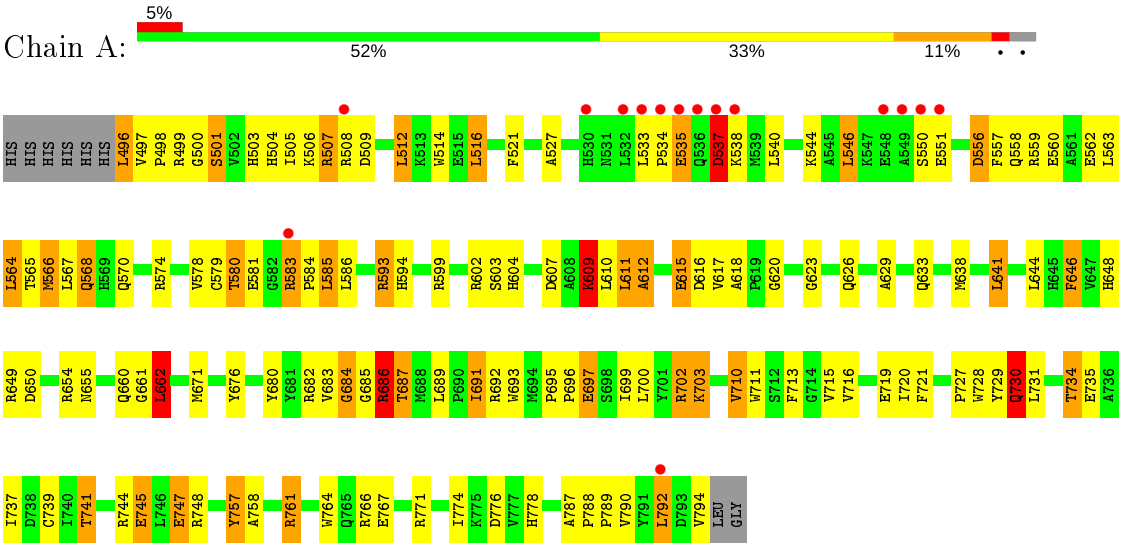
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	165	Total	O	0	0
			165	165		

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 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: Tyrosine-protein kinase receptor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	105.12Å 105.12Å 203.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.46 41.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	80.0 (19.90-2.46) 77.2 (41.56-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.236 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2553	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	1.70	33/2448 (1.3%)	1.37	26/3315 (0.8%)

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	747	GLU	CG-CD	11.27	1.68	1.51
1	A	719	GLU	CD-OE2	10.38	1.37	1.25
1	A	697	GLU	CG-CD	9.05	1.65	1.51
1	A	787	ALA	CA-CB	7.88	1.69	1.52
1	A	676	TYR	CD2-CE2	7.35	1.50	1.39
1	A	787	ALA	C-O	7.04	1.36	1.23
1	A	721	PHE	CD2-CE2	7.01	1.53	1.39
1	A	719	GLU	CG-CD	6.96	1.62	1.51
1	A	758	ALA	CA-CB	6.83	1.66	1.52
1	A	739	CYS	CB-SG	-6.71	1.70	1.82
1	A	693	TRP	CE3-CZ3	6.61	1.49	1.38
1	A	680	TYR	CG-CD1	6.55	1.47	1.39
1	A	715	VAL	CB-CG2	6.51	1.66	1.52
1	A	729	TYR	CE1-CZ	6.47	1.47	1.38
1	A	728	TRP	CB-CG	6.36	1.61	1.50
1	A	618	ALA	CA-CB	6.24	1.65	1.52
1	A	710	VAL	CB-CG1	-6.08	1.40	1.52
1	A	745	GLU	CG-CD	6.04	1.61	1.51
1	A	767	GLU	CG-CD	6.02	1.60	1.51
1	A	602	ARG	CZ-NH2	5.77	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603	SER	CB-OG	5.67	1.49	1.42
1	A	499	ARG	CG-CD	5.64	1.66	1.51
1	A	559	ARG	CG-CD	5.62	1.66	1.51
1	A	757	TYR	CD1-CE1	5.59	1.47	1.39
1	A	680	TYR	N-CA	5.55	1.57	1.46
1	A	730	GLN	CG-CD	5.46	1.63	1.51
1	A	757	TYR	CD2-CE2	5.39	1.47	1.39
1	A	728	TRP	CE3-CZ3	5.31	1.47	1.38
1	A	607	ASP	CB-CG	5.17	1.62	1.51
1	A	713	PHE	CE1-CZ	5.17	1.47	1.37
1	A	646	PHE	CB-CG	-5.15	1.42	1.51
1	A	514	TRP	CZ3-CH2	5.08	1.48	1.40
1	A	521	PHE	CB-CG	5.05	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	702	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	602	ARG	NE-CZ-NH1	-8.47	116.06	120.30
1	A	599	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	671	MET	CG-SD-CE	-7.75	87.80	100.20
1	A	602	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	A	641	LEU	CB-CG-CD2	-6.73	99.56	111.00
1	A	748	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	662	LEU	CB-CG-CD1	-6.51	99.93	111.00
1	A	654	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	689	LEU	CB-CG-CD2	6.41	121.90	111.00
1	A	583	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	710	VAL	CG1-CB-CG2	-5.93	101.41	110.90
1	A	702	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	516	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	792	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	761	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	787	ALA	CB-CA-C	5.56	118.44	110.10
1	A	609	LYS	CD-CE-NZ	5.52	124.39	111.70
1	A	546	LEU	CB-CG-CD2	-5.51	101.62	111.00
1	A	735	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	A	496	LEU	CB-CG-CD2	5.47	120.31	111.00
1	A	699	ILE	CG1-CB-CG2	-5.31	99.71	111.40
1	A	745	GLU	CA-CB-CG	5.11	124.65	113.40
1	A	771	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	599	ARG	NE-CZ-NH1	5.06	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	691	ILE	CA-CB-CG2	5.05	121.00	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	684	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	2388	0	2385	82	0
2	A	165	0	0	12	0
All	All	2553	0	2385	82	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 17.

All (82) 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:507:ARG:NH1	1:A:579:CYS:SG	2.02	1.32
1:A:703:LYS:HG3	2:A:935:HOH:O	1.46	1.12
1:A:500:GLY:O	1:A:501:SER:HB2	1.41	1.09
1:A:611:LEU:O	1:A:612:ALA:HB3	1.57	1.00
1:A:611:LEU:O	1:A:612:ALA:CB	2.09	0.99
1:A:686:ARG:HD2	1:A:686:ARG:O	1.66	0.94
1:A:684:GLY:HA3	1:A:687:THR:HG23	1.55	0.89
1:A:734:THR:CG2	2:A:879:HOH:O	2.20	0.88
1:A:737:ILE:O	1:A:741:THR:HB	1.72	0.88
1:A:745:GLU:OE2	1:A:761:ARG:NH1	2.07	0.87
1:A:500:GLY:O	1:A:501:SER:CB	2.18	0.85
1:A:649:ARG:HD3	2:A:896:HOH:O	1.81	0.80
1:A:609:LYS:HE3	1:A:609:LYS:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ARG:CD	1:A:686:ARG:O	2.30	0.79
1:A:686:ARG:C	1:A:686:ARG:CD	2.57	0.73
1:A:578:VAL:HG12	1:A:579:CYS:N	2.04	0.71
1:A:593:ARG:HG2	1:A:593:ARG:NH1	2.04	0.71
1:A:507:ARG:NH1	1:A:579:CYS:HG	1.88	0.69
1:A:593:ARG:HG2	1:A:593:ARG:HH11	1.56	0.69
1:A:578:VAL:CG1	1:A:579:CYS:N	2.56	0.68
1:A:682:ARG:CD	2:A:884:HOH:O	2.42	0.67
1:A:611:LEU:O	2:A:801:HOH:O	2.13	0.66
1:A:757:TYR:CE2	1:A:761:ARG:HD2	2.31	0.66
1:A:557:PHE:HE2	1:A:578:VAL:HG11	1.61	0.65
1:A:685:GLY:O	1:A:687:THR:N	2.28	0.65
1:A:623:GLY:H	1:A:626:GLN:HE21	1.45	0.64
1:A:560:GLU:O	1:A:564:LEU:HD22	2.00	0.62
1:A:686:ARG:CG	1:A:686:ARG:O	2.47	0.61
1:A:566:MET:HG3	1:A:567:LEU:N	2.13	0.61
1:A:648:HIS:O	1:A:649:ARG:HB2	2.00	0.61
1:A:682:ARG:HD3	2:A:884:HOH:O	2.00	0.61
1:A:716:VAL:O	1:A:720:ILE:HG13	2.00	0.61
1:A:593:ARG:CG	1:A:593:ARG:HH11	2.14	0.61
1:A:730:GLN:H	1:A:730:GLN:CD	2.04	0.60
1:A:507:ARG:NH2	1:A:584:PRO:O	2.36	0.59
1:A:686:ARG:C	1:A:686:ARG:HD2	2.20	0.59
1:A:557:PHE:CE2	1:A:578:VAL:HG11	2.37	0.58
1:A:506:LYS:O	1:A:509:ASP:N	2.38	0.56
1:A:734:THR:HG22	2:A:879:HOH:O	1.96	0.55
1:A:629:ALA:O	1:A:633:GLN:HG3	2.09	0.53
1:A:650:ASP:O	1:A:655:ASN:ND2	2.36	0.53
1:A:558:GLN:O	1:A:562:GLU:HG3	2.09	0.53
1:A:568:GLN:HG3	2:A:883:HOH:O	2.09	0.52
1:A:609:LYS:HA	1:A:609:LYS:CE	2.36	0.52
1:A:503:HIS:CE1	1:A:504:HIS:O	2.63	0.51
1:A:682:ARG:HD2	2:A:884:HOH:O	2.07	0.51
1:A:556:ASP:N	1:A:556:ASP:OD2	2.44	0.50
1:A:604:HIS:HD2	1:A:620:GLY:O	1.95	0.50
1:A:734:THR:HG21	2:A:928:HOH:O	2.11	0.50
1:A:683:VAL:HG23	1:A:684:GLY:N	2.27	0.49
1:A:503:HIS:ND1	1:A:504:HIS:O	2.46	0.48
1:A:638:MET:HB3	1:A:774:ILE:HG12	1.94	0.48
1:A:696:PRO:O	1:A:700:LEU:HG	2.13	0.48
1:A:578:VAL:CG1	1:A:579:CYS:H	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:PHE:CE1	1:A:585:LEU:HB3	2.48	0.48
1:A:695:PRO:HB2	1:A:697:GLU:OE1	2.13	0.48
1:A:535:GLU:H	1:A:535:GLU:CD	2.17	0.47
1:A:579:CYS:SG	1:A:581:GLU:HG2	2.55	0.47
1:A:527:ALA:O	1:A:540:LEU:HA	2.15	0.47
1:A:692:ARG:HD3	1:A:727:PRO:O	2.15	0.46
1:A:684:GLY:HA3	1:A:687:THR:CG2	2.38	0.46
1:A:644:LEU:HB3	1:A:646:PHE:HD2	1.79	0.46
1:A:512:LEU:HD12	1:A:527:ALA:HB2	1.98	0.46
1:A:504:HIS:C	1:A:505:ILE:HG13	2.35	0.46
1:A:506:LYS:O	1:A:507:ARG:C	2.54	0.45
1:A:661:GLY:O	1:A:662:LEU:CB	2.64	0.45
1:A:580:THR:HA	1:A:585:LEU:HD12	1.98	0.45
1:A:533:LEU:HA	1:A:534:PRO:HD3	1.85	0.44
1:A:550:SER:O	1:A:551:GLU:C	2.56	0.44
1:A:594:HIS:HE1	1:A:616:ASP:OD1	1.99	0.44
1:A:544:LYS:O	1:A:586:LEU:HA	2.19	0.43
1:A:660:GLN:NE2	2:A:805:HOH:O	2.41	0.43
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.64	0.42
1:A:537:ASP:CG	1:A:538:LYS:N	2.73	0.42
1:A:503:HIS:HD1	1:A:504:HIS:N	2.17	0.42
1:A:593:ARG:NH2	1:A:615:GLU:OE1	2.53	0.42
1:A:778:HIS:HD2	2:A:922:HOH:O	2.03	0.42
1:A:730:GLN:N	1:A:730:GLN:OE1	2.53	0.41
1:A:686:ARG:C	1:A:686:ARG:HD3	2.40	0.41
1:A:563:LEU:HD12	1:A:566:MET:HG2	2.01	0.41
1:A:711:TRP:CE3	1:A:764:TRP:HA	2.56	0.40
1:A:788:PRO:HA	1:A:789:PRO:HD2	1.88	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	297/307 (97%)	277 (93%)	15 (5%)	5 (2%)	9 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	686	ARG
1	A	501	SER
1	A	537	ASP
1	A	612	ALA
1	A	792	LEU

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	251/258 (97%)	208 (83%)	43 (17%)	2 1

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	LEU
1	A	497	VAL
1	A	498	PRO
1	A	507	ARG
1	A	508	ARG
1	A	512	LEU
1	A	516	LEU
1	A	535	GLU
1	A	537	ASP
1	A	546	LEU
1	A	556	ASP
1	A	564	LEU
1	A	565	THR
1	A	566	MET
1	A	568	GLN
1	A	570	GLN

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Mol	Chain	Res	Type
1	A	574	ARG
1	A	580	THR
1	A	583	ARG
1	A	585	LEU
1	A	593	ARG
1	A	609	LYS
1	A	610	LEU
1	A	611	LEU
1	A	615	GLU
1	A	617	VAL
1	A	662	LEU
1	A	686	ARG
1	A	687	THR
1	A	691	ILE
1	A	702	ARG
1	A	703	LYS
1	A	710	VAL
1	A	730	GLN
1	A	731	LEU
1	A	734	THR
1	A	741	THR
1	A	744	ARG
1	A	747	GLU
1	A	766	ARG
1	A	776	ASP
1	A	790	VAL
1	A	794	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	GLN
1	A	594	HIS
1	A	604	HIS
1	A	626	GLN
1	A	778	HIS

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	299/307 (97%)	0.06	15 (5%)	28	26	16, 32, 67, 80	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	792	LEU	4.8
1	A	537	ASP	4.1
1	A	534	PRO	4.1
1	A	538	LYS	3.8
1	A	551	GLU	3.6
1	A	533	LEU	3.1
1	A	550	SER	3.1
1	A	583	ARG	3.0
1	A	530	HIS	2.9
1	A	549	ALA	2.7
1	A	548	GLU	2.6
1	A	536	GLN	2.4
1	A	535	GLU	2.4
1	A	532	LEU	2.3
1	A	508	ARG	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.