Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 11:28 PM EDT

PDB ID	:	3P6A
Title	:	Crystal Structure of the DH/PH domains of p115-RhoGEF (R399E mutant)
Authors	:	Chen, Z.; Guo, L.; Sprang, S.R.; Sternweis, P.C.
Deposited on	:	2010-10-11
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

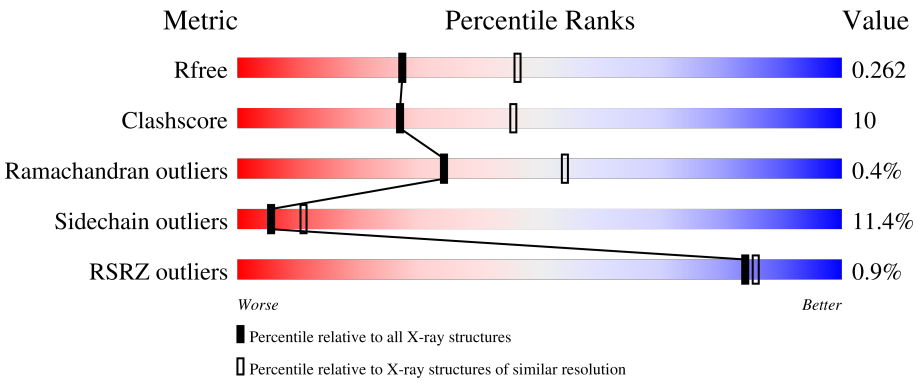
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 >=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	377	.% 66% 18% 7% 9%
1	B	377	66% 20% 5% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5653 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	2832	1792	509	515	16	0	0	0
1	B	343	2821	1786	505	514	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

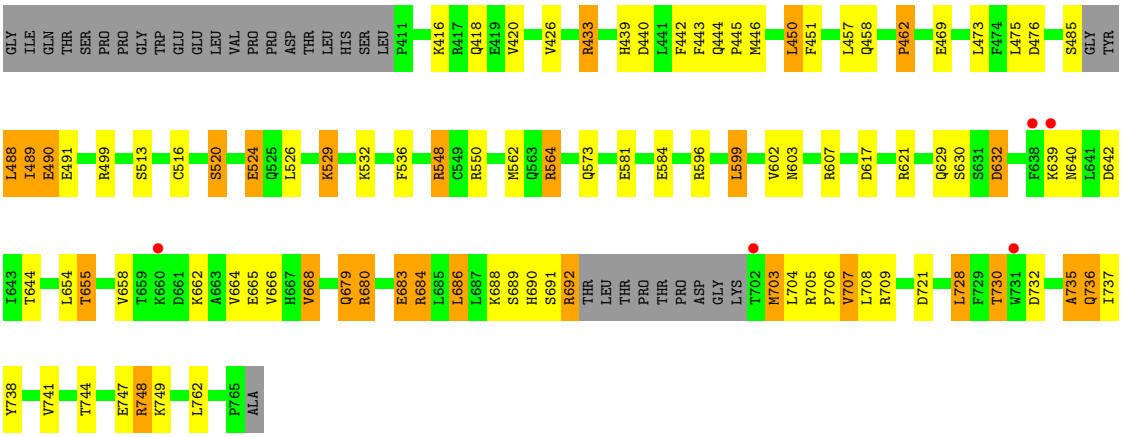
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	GLY	-	expression tag	UNP Q92888
A	391	ILE	-	expression tag	UNP Q92888
A	392	GLN	-	expression tag	UNP Q92888
A	393	THR	-	expression tag	UNP Q92888
A	394	SER	-	expression tag	UNP Q92888
A	399	GLU	ARG	engineered mutation	UNP Q92888
B	390	GLY	-	expression tag	UNP Q92888
B	391	ILE	-	expression tag	UNP Q92888
B	392	GLN	-	expression tag	UNP Q92888
B	393	THR	-	expression tag	UNP Q92888
B	394	SER	-	expression tag	UNP Q92888
B	399	GLU	ARG	engineered mutation	UNP Q92888

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.

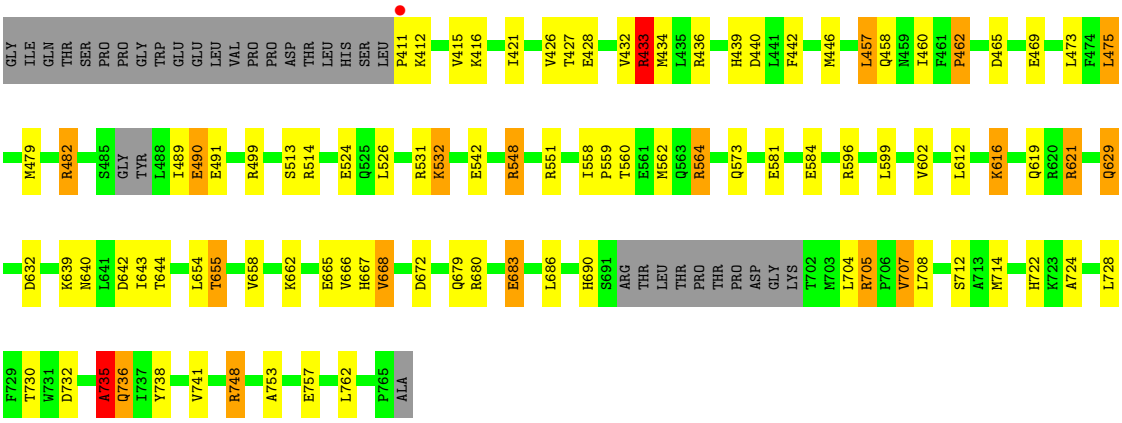
• Molecule 1: Rho guanine nucleotide exchange factor 1

Chain A:



• Molecule 1: Rho guanine nucleotide exchange factor 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	110.82Å 110.82Å 98.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.30 – 2.50 48.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.30-2.50) 99.8 (48.30-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.226 , 0.266 0.223 , 0.262	Depositor DCC
R_{free} test set	2372 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 10.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.478 for h,-h-k,-l 0.011 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5653	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 (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	A	1.08	4/2879 (0.1%)	1.06	14/3874 (0.4%)
1	B	1.10	3/2868 (0.1%)	1.03	12/3860 (0.3%)
All	All	1.09	7/5747 (0.1%)	1.05	26/7734 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	469	GLU	CG-CD	6.82	1.62	1.51
1	B	524	GLU	CG-CD	6.39	1.61	1.51
1	A	516	CYS	CB-SG	-6.06	1.72	1.82
1	A	469	GLU	CG-CD	5.96	1.60	1.51
1	A	524	GLU	CD-OE1	5.54	1.31	1.25
1	B	524	GLU	CD-OE2	5.21	1.31	1.25
1	A	520	SER	CB-OG	-5.20	1.35	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	499	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	564	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	564	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	714	MET	CG-SD-CE	-7.21	88.66	100.20
1	A	499	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	450	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	462	PRO	C-N-CA	-6.98	104.26	121.70
1	B	499	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	433	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	680	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	562	MET	CG-SD-CE	-6.22	90.24	100.20
1	B	457	LEU	CB-CG-CD1	-6.04	100.74	111.00
1	A	748	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	735	ALA	C-N-CA	5.84	136.31	121.70
1	B	433	ARG	NE-CZ-NH2	-5.81	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	748	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	562	MET	CG-SD-CE	-5.61	91.22	100.20
1	A	476	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	462	PRO	C-N-CA	-5.47	108.03	121.70
1	A	721	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	465	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	469	GLU	OE1-CD-OE2	-5.28	116.97	123.30
1	B	434	MET	CG-SD-CE	5.24	108.58	100.20
1	A	728	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	482	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	735	ALA	C-N-CA	5.07	134.36	121.70

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	A	2832	0	2895	65	0
1	B	2821	0	2882	55	0
All	All	5653	0	5777	116	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 10.

All (116) 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:639:LYS:HG3	1:A:640:ASN:HB2	1.13	1.08
1:A:639:LYS:CG	1:A:640:ASN:HB2	1.88	1.04
1:B:548:ARG:HH11	1:B:548:ARG:HG2	1.21	1.01
1:A:684:ARG:HH11	1:A:684:ARG:HG2	1.27	0.98
1:B:705:ARG:HH11	1:B:705:ARG:HG3	1.28	0.97
1:A:548:ARG:HH11	1:A:548:ARG:HG2	1.32	0.94
1:B:433:ARG:HH11	1:B:433:ARG:HG2	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:ARG:HH11	1:B:705:ARG:CG	1.84	0.91
1:B:619:GLN:HE21	1:B:643:ILE:H	1.28	0.82
1:A:732:ASP:OD2	1:A:736:GLN:CB	2.29	0.79
1:A:485:SER:HB2	1:A:489:ILE:HG22	1.65	0.79
1:A:485:SER:CB	1:A:489:ILE:HG22	2.13	0.78
1:A:688:LYS:HE2	1:A:690:HIS:HB3	1.68	0.76
1:A:573:GLN:HE21	1:A:596:ARG:HH21	1.33	0.76
1:A:684:ARG:HG2	1:A:684:ARG:NH1	1.99	0.69
1:B:489:ILE:O	1:B:490:GLU:HB3	1.90	0.69
1:A:639:LYS:HG3	1:A:640:ASN:CB	2.07	0.68
1:B:619:GLN:NE2	1:B:643:ILE:H	1.91	0.68
1:B:705:ARG:HG3	1:B:705:ARG:NH1	2.02	0.67
1:A:439:HIS:HD2	1:A:440:ASP:OD2	1.79	0.66
1:B:712:SER:HB2	1:B:730:THR:HB	1.78	0.65
1:A:732:ASP:OD2	1:A:736:GLN:HG3	1.97	0.65
1:A:730:THR:HG21	1:B:433:ARG:HH22	1.62	0.65
1:B:548:ARG:HG2	1:B:548:ARG:NH1	2.02	0.64
1:B:732:ASP:OD2	1:B:736:GLN:HB3	1.97	0.63
1:B:421:ILE:HG21	1:B:489:ILE:HD12	1.81	0.63
1:A:732:ASP:OD2	1:A:736:GLN:CG	2.49	0.61
1:A:691:SER:CB	1:A:704:LEU:H	2.13	0.61
1:B:442:PHE:O	1:B:446:MET:HG3	1.99	0.60
1:A:654:LEU:HD12	1:A:668:VAL:HG11	1.83	0.60
1:B:621:ARG:HD2	1:B:683:GLU:O	2.03	0.59
1:A:639:LYS:CB	1:A:640:ASN:HB2	2.32	0.59
1:B:427:THR:OG1	1:B:564:ARG:NH2	2.35	0.59
1:A:642:ASP:OD1	1:A:644:THR:HB	2.02	0.59
1:A:548:ARG:HH11	1:A:548:ARG:CG	2.10	0.59
1:A:529:LYS:HB3	1:A:536:PHE:CD2	2.38	0.58
1:A:418:GLN:HE22	1:A:489:ILE:HG12	1.67	0.58
1:A:730:THR:HG21	1:B:433:ARG:NH2	2.18	0.58
1:A:442:PHE:O	1:A:446:MET:HG3	2.05	0.57
1:A:689:SER:HA	1:A:706:PRO:HD3	1.87	0.57
1:B:722:HIS:O	1:B:748:ARG:HD3	2.05	0.56
1:B:619:GLN:HE21	1:B:643:ILE:HG12	1.71	0.56
1:A:732:ASP:OD2	1:A:736:GLN:HB3	2.05	0.55
1:B:642:ASP:OD1	1:B:644:THR:HB	2.06	0.55
1:B:489:ILE:O	1:B:490:GLU:CB	2.55	0.55
1:B:548:ARG:HH11	1:B:548:ARG:CG	2.03	0.55
1:A:655:THR:HB	1:A:665:GLU:OE2	2.08	0.54
1:A:737:ILE:HD12	1:B:482:ARG:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:LYS:HB2	1:B:640:ASN:HB2	1.89	0.54
1:A:735:ALA:HA	1:A:736:GLN:HB2	1.88	0.54
1:A:664:VAL:HG13	1:A:679:GLN:OE1	2.09	0.53
1:B:573:GLN:HE21	1:B:596:ARG:HH21	1.56	0.52
1:B:458:GLN:O	1:B:462:PRO:HA	2.09	0.52
1:A:599:LEU:HD22	1:A:603:ASN:ND2	2.24	0.52
1:A:621:ARG:HD2	1:A:683:GLU:O	2.09	0.52
1:B:513:SER:HB2	1:B:602:VAL:HG22	1.92	0.52
1:B:428:GLU:OE1	1:B:564:ARG:NH1	2.42	0.52
1:A:691:SER:O	1:A:692:ARG:O	2.27	0.51
1:A:738:TYR:CD1	1:A:738:TYR:N	2.78	0.51
1:B:432:VAL:O	1:B:436:ARG:HG2	2.11	0.51
1:B:724:ALA:O	1:B:748:ARG:HD2	2.11	0.51
1:A:488:LEU:C	1:A:488:LEU:HD22	2.31	0.50
1:A:735:ALA:CA	1:A:736:GLN:HB2	2.41	0.50
1:B:439:HIS:HD2	1:B:440:ASP:OD2	1.93	0.50
1:A:451:PHE:O	1:A:529:LYS:HE3	2.12	0.50
1:B:654:LEU:HD12	1:B:668:VAL:HG11	1.94	0.50
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.93	0.50
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.77	0.50
1:A:617:ASP:O	1:A:621:ARG:HG3	2.11	0.50
1:A:691:SER:OG	1:A:703:MET:N	2.45	0.49
1:A:737:ILE:HD12	1:B:482:ARG:HG2	1.94	0.49
1:B:475:LEU:HD22	1:B:479:MET:SD	2.53	0.49
1:B:491:GLU:HA	1:B:584:GLU:CD	2.33	0.49
1:B:735:ALA:CA	1:B:736:GLN:HB2	2.43	0.49
1:A:744:THR:OG1	1:A:747:GLU:HB2	2.13	0.49
1:A:690:HIS:CG	1:A:690:HIS:O	2.65	0.49
1:A:632:ASP:OD2	1:A:705:ARG:NH1	2.46	0.49
1:B:738:TYR:N	1:B:738:TYR:CD1	2.81	0.49
1:A:732:ASP:OD2	1:A:736:GLN:HB2	2.11	0.48
1:B:433:ARG:HG2	1:B:433:ARG:NH1	2.09	0.48
1:B:707:VAL:C	1:B:708:LEU:HG	2.33	0.48
1:B:667:HIS:CD2	1:B:680:ARG:HH21	2.32	0.48
1:A:686:LEU:HD23	1:A:688:LYS:HG3	1.96	0.47
1:A:458:GLN:O	1:A:462:PRO:HA	2.14	0.47
1:B:433:ARG:HH11	1:B:433:ARG:CG	2.15	0.47
1:B:612:LEU:O	1:B:616:LYS:HB2	2.15	0.47
1:B:629:GLN:O	1:B:629:GLN:HG2	2.14	0.46
1:A:573:GLN:HE21	1:A:596:ARG:NH2	2.09	0.45
1:A:689:SER:O	1:A:704:LEU:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLU:HA	1:A:584:GLU:CD	2.38	0.45
1:B:655:THR:HB	1:B:665:GLU:OE2	2.17	0.45
1:A:703:MET:H	1:A:703:MET:HG2	1.32	0.44
1:A:513:SER:HB2	1:A:602:VAL:HG22	2.00	0.44
1:A:573:GLN:NE2	1:A:596:ARG:HH21	2.09	0.44
1:A:416:LYS:O	1:A:420:VAL:HG23	2.18	0.44
1:B:619:GLN:NE2	1:B:642:ASP:HA	2.33	0.43
1:B:735:ALA:N	1:B:736:GLN:HB2	2.32	0.43
1:A:520:SER:O	1:A:524:GLU:HG2	2.19	0.43
1:B:532:LYS:HD3	1:B:532:LYS:C	2.39	0.43
1:A:439:HIS:HA	1:A:443:PHE:HB3	2.01	0.43
1:A:684:ARG:NH1	1:A:684:ARG:CG	2.77	0.43
1:B:732:ASP:OD2	1:B:736:GLN:CB	2.66	0.43
1:A:707:VAL:C	1:A:708:LEU:HG	2.38	0.42
1:A:490:GLU:O	1:A:491:GLU:HB2	2.19	0.42
1:B:632:ASP:OD2	1:B:705:ARG:NH1	2.52	0.42
1:A:607:ARG:HG2	1:A:607:ARG:NH1	2.35	0.42
1:A:607:ARG:HG2	1:A:607:ARG:HH11	1.85	0.42
1:B:460:ILE:C	1:B:462:PRO:HD3	2.40	0.41
1:B:704:LEU:CD2	1:B:736:GLN:OE1	2.68	0.41
1:B:558:ILE:N	1:B:559:PRO:CD	2.84	0.41
1:B:753:ALA:O	1:B:757:GLU:HG3	2.20	0.41
1:A:630:SER:OG	1:A:632:ASP:HB3	2.21	0.41
1:B:662:LYS:NZ	1:B:690:HIS:HD2	2.19	0.41
1:A:658:VAL:HG22	1:A:662:LYS:HB3	2.03	0.41
1:B:679:GLN:NE2	1:B:690:HIS:HE1	2.19	0.40
1:A:664:VAL:HG21	1:A:690:HIS:NE2	2.36	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	338/377 (90%)	320 (95%)	17 (5%)	1 (0%)	41	61
1	B	337/377 (89%)	322 (96%)	13 (4%)	2 (1%)	25	43
All	All	675/754 (90%)	642 (95%)	30 (4%)	3 (0%)	34	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	GLN
1	B	736	GLN
1	B	735	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	317/346 (92%)	281 (89%)	36 (11%)	5	11
1	B	316/346 (91%)	280 (89%)	36 (11%)	5	11
All	All	633/692 (92%)	561 (89%)	72 (11%)	5	11

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	426	VAL
1	A	450	LEU
1	A	457	LEU
1	A	473	LEU
1	A	475	LEU
1	A	488	LEU
1	A	489	ILE
1	A	490	GLU
1	A	526	LEU
1	A	529	LYS
1	A	532	LYS
1	A	548	ARG
1	A	550	ARG

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Mol	Chain	Res	Type
1	A	564	ARG
1	A	581	GLU
1	A	599	LEU
1	A	629	GLN
1	A	632	ASP
1	A	655	THR
1	A	666	VAL
1	A	668	VAL
1	A	679	GLN
1	A	680	ARG
1	A	683	GLU
1	A	684	ARG
1	A	686	LEU
1	A	692	ARG
1	A	703	MET
1	A	707	VAL
1	A	709	ARG
1	A	728	LEU
1	A	730	THR
1	A	741	VAL
1	A	748	ARG
1	A	749	LYS
1	A	762	LEU
1	B	411	PRO
1	B	412	LYS
1	B	415	VAL
1	B	416	LYS
1	B	426	VAL
1	B	433	ARG
1	B	457	LEU
1	B	473	LEU
1	B	475	LEU
1	B	490	GLU
1	B	514	ARG
1	B	526	LEU
1	B	531	ARG
1	B	532	LYS
1	B	542	GLU
1	B	548	ARG
1	B	551	ARG
1	B	560	THR
1	B	564	ARG

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Mol	Chain	Res	Type
1	B	581	GLU
1	B	599	LEU
1	B	616	LYS
1	B	621	ARG
1	B	629	GLN
1	B	655	THR
1	B	658	VAL
1	B	666	VAL
1	B	668	VAL
1	B	672	ASP
1	B	683	GLU
1	B	686	LEU
1	B	705	ARG
1	B	707	VAL
1	B	728	LEU
1	B	741	VAL
1	B	762	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	439	HIS
1	A	444	GLN
1	A	459	ASN
1	A	541	GLN
1	A	573	GLN
1	A	601	HIS
1	A	629	GLN
1	B	414	GLN
1	B	439	HIS
1	B	541	GLN
1	B	573	GLN
1	B	601	HIS
1	B	604	GLN
1	B	619	GLN
1	B	667	HIS
1	B	679	GLN
1	B	690	HIS
1	B	733	GLN
1	B	750	ASN

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 monosaccharides 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	A	344/377 (91%)	0.07	5 (1%)	73	75	26, 44, 84, 110	0
1	B	343/377 (90%)	0.05	1 (0%)	94	94	25, 44, 82, 108	0
All	All	687/754 (91%)	0.06	6 (0%)	84	86	25, 44, 82, 110	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	702	THR	3.1
1	A	731	TRP	3.1
1	A	638	PHE	2.4
1	A	639	LYS	2.3
1	A	660	LYS	2.0
1	B	411	PRO	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 monosaccharides 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.