



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:42 am BST

PDB ID : 3ODO
Title : Crystal Structure of the DH/PH Domains of p115-RhoGEF
Authors : Chen, Z.; Guo, L.; Sprang, S.R.; Sternweis, P.C.
Deposited on : 2010-08-11
Resolution : 2.90 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

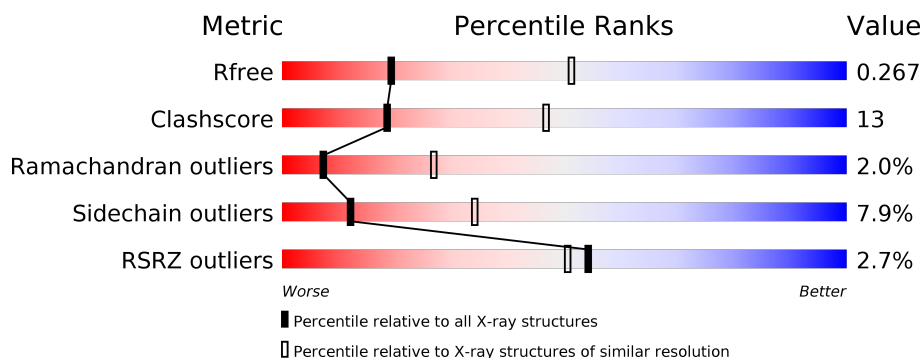
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	375	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
1	B	375	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>6%</div> <div>• •</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6068 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
1	A	370	Total	C	N	O	S	0	0	0
			3034	1919	542	557	16			
1	B	370	Total	C	N	O	S	0	0	0
			3034	1919	542	557	16			

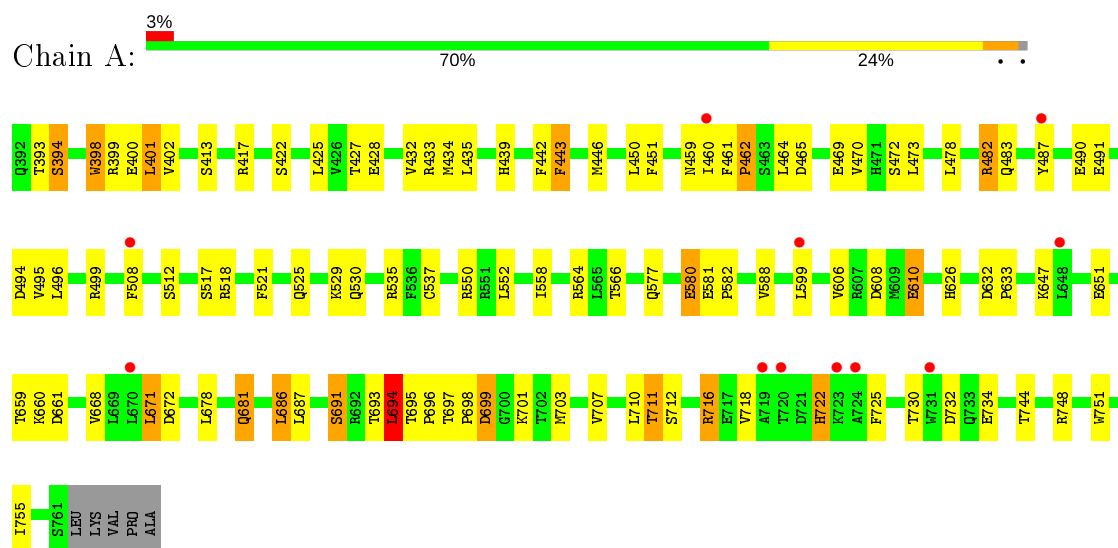
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLN	-	EXPRESSION TAG	UNP Q92888
A	393	THR	-	EXPRESSION TAG	UNP Q92888
A	394	SER	-	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

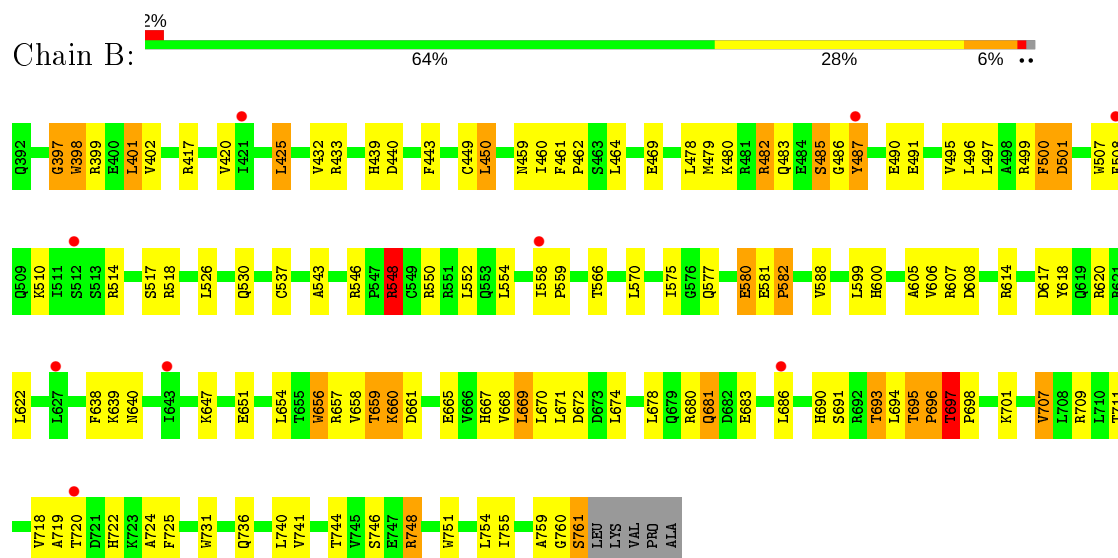
3 Residue-property plots [i](#)

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: Rho guanine nucleotide exchange factor 1



- Molecule 1: Rho guanine nucleotide exchange factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	106.05Å 106.05Å 125.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 2.90 35.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.00-2.90) 99.1 (35.94-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.221 , 0.272 0.220 , 0.267	Depositor DCC
R_{free} test set	1550 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6068	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.87	2/3092 (0.1%)	0.87	2/4176 (0.0%)
1	B	0.89	3/3092 (0.1%)	0.92	7/4176 (0.2%)
All	All	0.88	5/6184 (0.1%)	0.90	9/8352 (0.1%)

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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	665	GLU	CG-CD	7.61	1.63	1.51
1	B	681	GLN	CD-OE1	5.51	1.36	1.24
1	A	483	GLN	CD-OE1	5.48	1.36	1.24
1	A	681	GLN	CD-OE1	5.23	1.35	1.24
1	B	697	THR	CA-CB	5.13	1.66	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	LEU	CA-CB-CG	8.17	134.08	115.30
1	B	482	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	548	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	402	VAL	N-CA-C	-5.87	95.16	111.00
1	A	686	LEU	CA-CB-CG	5.77	128.57	115.30
1	B	425	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	A	694	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	482	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	665	GLU	OE1-CD-OE2	-5.08	117.21	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	695	THR	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	3034	0	3085	72	1
1	B	3034	0	3085	90	1
All	All	6068	0	6170	161	1

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 (161) 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:696:PRO:HA	1:A:697:THR:HB	1.36	1.05
1:B:425:LEU:HD21	1:B:482:ARG:HD2	1.38	1.04
1:A:718:VAL:HG23	1:A:725:PHE:HA	1.41	1.03
1:B:659:THR:HG21	1:B:694:LEU:HB3	1.53	0.89
1:B:718:VAL:HG23	1:B:725:PHE:HA	1.57	0.86
1:B:693:THR:OG1	1:B:695:THR:HG22	1.76	0.85
1:B:659:THR:HB	1:B:661:ASP:H	1.45	0.82
1:A:718:VAL:HG23	1:A:725:PHE:CA	2.10	0.80
1:B:638:PHE:O	1:B:639:LYS:HG2	1.81	0.79
1:B:425:LEU:CD2	1:B:482:ARG:HD2	2.18	0.73
1:A:439:HIS:HB2	1:A:464:LEU:HD21	1.71	0.72
1:B:656:TRP:HB3	1:B:740:LEU:HD13	1.71	0.72
1:A:517:SER:HA	1:A:606:VAL:HG22	1.72	0.72
1:A:580:GLU:CD	1:A:580:GLU:H	1.92	0.71
1:A:659:THR:HG22	1:A:660:LYS:N	2.06	0.71
1:A:659:THR:HG22	1:A:660:LYS:H	1.54	0.71
1:A:696:PRO:CA	1:A:697:THR:HB	2.18	0.71
1:B:695:THR:HG23	1:B:698:PRO:HD2	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:VAL:HG23	1:B:725:PHE:CA	2.22	0.70
1:B:693:THR:O	1:B:696:PRO:HB3	1.94	0.68
1:B:695:THR:HG23	1:B:696:PRO:HA	1.76	0.68
1:B:417:ARG:HH22	1:B:491:GLU:H	1.41	0.68
1:B:580:GLU:CD	1:B:580:GLU:H	1.96	0.68
1:B:459:ASN:O	1:B:518:ARG:HD3	1.94	0.67
1:B:659:THR:CG2	1:B:694:LEU:HB3	2.24	0.67
1:A:659:THR:HG21	1:A:694:LEU:HB2	1.76	0.66
1:B:548:ARG:HH11	1:B:548:ARG:HG2	1.60	0.66
1:B:499:ARG:NH1	1:B:508:PHE:HB2	2.10	0.66
1:A:434:MET:HE2	1:A:435:LEU:HG	1.78	0.65
1:A:499:ARG:O	1:A:499:ARG:HD3	1.97	0.64
1:B:478:LEU:HD23	1:B:495:VAL:HG11	1.79	0.64
1:B:605:ALA:O	1:B:608:ASP:HB2	1.98	0.63
1:B:724:ALA:HB2	1:B:741:VAL:HG13	1.83	0.61
1:A:496:LEU:HD12	1:A:588:VAL:HG22	1.83	0.60
1:A:722:HIS:N	1:A:722:HIS:ND1	2.49	0.60
1:B:638:PHE:C	1:B:639:LYS:HG2	2.22	0.60
1:A:470:VAL:CG1	1:A:508:PHE:HD1	2.15	0.60
1:B:401:LEU:O	1:B:401:LEU:HD12	2.02	0.59
1:A:659:THR:HG21	1:A:694:LEU:CB	2.32	0.59
1:B:517:SER:HA	1:B:606:VAL:HG22	1.83	0.59
1:B:669:LEU:HD22	1:B:678:LEU:HD11	1.84	0.59
1:A:478:LEU:HD12	1:A:495:VAL:HG11	1.85	0.58
1:B:660:LYS:HE3	1:B:660:LYS:HA	1.83	0.58
1:B:731:TRP:HZ3	1:B:736:GLN:HG2	1.68	0.58
1:A:698:PRO:O	1:A:699:ASP:HB2	2.03	0.58
1:B:722:HIS:O	1:B:748:ARG:HD3	2.04	0.57
1:B:510:LYS:HE3	1:B:514:ARG:NH2	2.21	0.56
1:B:659:THR:HG21	1:B:694:LEU:CB	2.29	0.55
1:A:701:LYS:NZ	1:B:552:LEU:O	2.39	0.55
1:A:428:GLU:N	1:A:564:ARG:NH2	2.55	0.55
1:A:459:ASN:O	1:A:518:ARG:HD3	2.06	0.55
1:B:443:PHE:HD1	1:B:461:PHE:HD2	1.55	0.54
1:B:548:ARG:NH1	1:B:548:ARG:HG2	2.21	0.54
1:B:669:LEU:HB3	1:B:671:LEU:HD13	1.90	0.54
1:B:443:PHE:HD1	1:B:461:PHE:CD2	2.27	0.52
1:B:480:LYS:O	1:B:483:GLN:HB3	2.10	0.52
1:B:566:THR:HG22	1:B:599:LEU:HD21	1.91	0.52
1:B:639:LYS:HB2	1:B:640:ASN:HB2	1.91	0.52
1:A:417:ARG:HH22	1:A:491:GLU:H	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:PRO:HA	1:A:697:THR:CB	2.12	0.52
1:B:660:LYS:HA	1:B:660:LYS:CE	2.40	0.52
1:B:751:TRP:O	1:B:755:ILE:HG13	2.10	0.50
1:A:478:LEU:CD1	1:A:495:VAL:HG11	2.41	0.50
1:B:425:LEU:HD21	1:B:482:ARG:CD	2.27	0.50
1:A:401:LEU:HD11	1:A:482:ARG:HH21	1.75	0.50
1:A:425:LEU:HD22	1:A:482:ARG:HD2	1.94	0.50
1:B:486:GLY:O	1:B:487:TYR:HB2	2.11	0.50
1:B:718:VAL:HG12	1:B:720:THR:HB	1.93	0.50
1:B:759:ALA:O	1:B:761:SER:N	2.45	0.49
1:B:731:TRP:CZ3	1:B:736:GLN:HG2	2.47	0.49
1:B:566:THR:HA	1:B:599:LEU:HD22	1.93	0.49
1:A:626:HIS:CE1	1:A:686:LEU:HD11	2.48	0.48
1:A:432:VAL:HG21	1:A:472:SER:HA	1.95	0.48
1:A:660:LYS:HE2	1:A:660:LYS:HA	1.94	0.48
1:B:482:ARG:O	1:B:485:SER:O	2.31	0.48
1:B:439:HIS:HB2	1:B:464:LEU:HD21	1.95	0.47
1:B:550:ARG:HG3	1:B:550:ARG:O	2.15	0.47
1:A:698:PRO:O	1:A:699:ASP:CB	2.62	0.47
1:B:469:GLU:HA	1:B:469:GLU:OE1	2.15	0.47
1:A:443:PHE:HD1	1:A:461:PHE:HD2	1.62	0.47
1:A:710:LEU:O	1:A:711:THR:C	2.53	0.47
1:A:442:PHE:O	1:A:446:MET:HG3	2.15	0.46
1:A:722:HIS:O	1:A:748:ARG:HD3	2.15	0.46
1:A:428:GLU:CA	1:A:564:ARG:HH21	2.29	0.46
1:B:496:LEU:HD12	1:B:588:VAL:HG22	1.96	0.46
1:B:558:ILE:HB	1:B:559:PRO:HD3	1.97	0.46
1:A:716:ARG:HG2	1:A:716:ARG:HH11	1.80	0.46
1:B:543:ALA:O	1:B:546:ARG:HG3	2.16	0.46
1:B:674:LEU:HD23	1:B:707:VAL:HG23	1.98	0.46
1:B:490:GLU:O	1:B:491:GLU:HB3	2.15	0.46
1:B:696:PRO:HA	1:B:697:THR:HA	1.73	0.46
1:B:659:THR:HB	1:B:661:ASP:N	2.23	0.45
1:A:460:ILE:C	1:A:462:PRO:HD3	2.36	0.45
1:B:440:ASP:OD2	1:B:548:ARG:NH2	2.49	0.45
1:B:581:GLU:HA	1:B:582:PRO:HD2	1.72	0.45
1:A:691:SER:HA	1:A:703:MET:HG2	1.98	0.45
1:A:428:GLU:CA	1:A:564:ARG:NH2	2.79	0.45
1:A:678:LEU:HD23	1:A:687:LEU:CD2	2.46	0.45
1:A:751:TRP:O	1:A:755:ILE:HG13	2.17	0.45
1:B:667:HIS:CG	1:B:680:ARG:HH21	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:C	1:A:400:GLU:N	2.68	0.44
1:A:425:LEU:HD21	1:A:482:ARG:HD3	1.99	0.44
1:A:490:GLU:O	1:A:491:GLU:HB3	2.17	0.44
1:A:451:PHE:HB3	1:A:529:LYS:HE2	1.99	0.44
1:A:393:THR:HG23	1:A:433:ARG:NH1	2.32	0.44
1:B:617:ASP:HA	1:B:620:ARG:NH2	2.33	0.44
1:B:449:CYS:O	1:B:450:LEU:HD12	2.17	0.44
1:A:660:LYS:HE2	1:A:660:LYS:CA	2.47	0.44
1:A:427:THR:OG1	1:A:564:ARG:NH1	2.50	0.43
1:A:671:LEU:HA	1:A:671:LEU:HD12	1.77	0.43
1:B:659:THR:HG22	1:B:660:LYS:H	1.82	0.43
1:A:632:ASP:OD1	1:A:633:PRO:HD2	2.19	0.43
1:A:566:THR:HA	1:A:599:LEU:HD22	2.01	0.43
1:A:647:LYS:HB3	1:A:672:ASP:HB3	2.01	0.43
1:A:678:LEU:HD23	1:A:687:LEU:HD21	2.01	0.43
1:B:397:GLY:O	1:B:398:TRP:HB2	2.19	0.43
1:A:469:GLU:HA	1:A:469:GLU:OE2	2.19	0.42
1:A:402:VAL:O	1:A:402:VAL:HG13	2.18	0.42
1:B:510:LYS:HE3	1:B:514:ARG:HH22	1.84	0.42
1:B:420:VAL:HG12	1:B:575:ILE:HG13	2.01	0.42
1:B:606:VAL:HG12	1:B:607:ARG:N	2.34	0.42
1:A:443:PHE:HD1	1:A:461:PHE:CD2	2.37	0.42
1:A:428:GLU:OE1	1:A:564:ARG:NH2	2.52	0.42
1:B:654:LEU:HD11	1:B:751:TRP:NE1	2.35	0.42
1:B:639:LYS:H	1:B:640:ASN:C	2.23	0.42
1:B:696:PRO:HA	1:B:698:PRO:HD2	2.00	0.42
1:B:719:ALA:O	1:B:720:THR:C	2.58	0.42
1:B:759:ALA:C	1:B:761:SER:H	2.23	0.42
1:A:428:GLU:HA	1:A:564:ARG:HH21	1.85	0.42
1:B:439:HIS:HB2	1:B:464:LEU:CD2	2.49	0.42
1:B:496:LEU:O	1:B:500:PHE:HB2	2.20	0.42
1:B:651:GLU:HA	1:B:668:VAL:O	2.20	0.42
1:B:718:VAL:CG1	1:B:720:THR:HB	2.49	0.42
1:A:530:GLN:HG3	1:A:537:CYS:HA	2.01	0.41
1:A:651:GLU:HA	1:A:668:VAL:O	2.20	0.41
1:B:432:VAL:O	1:B:433:ARG:C	2.57	0.41
1:A:425:LEU:CD2	1:A:482:ARG:HD3	2.49	0.41
1:A:550:ARG:O	1:A:550:ARG:HG3	2.18	0.41
1:B:696:PRO:HD2	1:B:696:PRO:O	2.20	0.41
1:B:658:VAL:HG11	1:B:690:HIS:HB3	2.01	0.41
1:B:497:LEU:O	1:B:501:ASP:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:LYS:HB3	1:B:672:ASP:HB3	2.01	0.41
1:A:712:SER:HB2	1:A:730:THR:H	1.85	0.41
1:B:479:MET:O	1:B:483:GLN:HB2	2.20	0.41
1:A:464:LEU:O	1:A:465:ASP:C	2.58	0.41
1:B:499:ARG:O	1:B:500:PHE:CG	2.74	0.41
1:B:526:LEU:HD13	1:B:554:LEU:HD21	2.03	0.41
1:A:393:THR:HG23	1:A:394:SER:N	2.35	0.41
1:B:530:GLN:HG3	1:B:537:CYS:HA	2.02	0.41
1:A:402:VAL:O	1:A:402:VAL:CG1	2.68	0.41
1:A:581:GLU:HA	1:A:582:PRO:HD2	1.97	0.41
1:B:499:ARG:HH22	1:B:507:TRP:HD1	1.69	0.41
1:A:469:GLU:O	1:A:473:LEU:HG	2.20	0.41
1:B:570:LEU:HA	1:B:570:LEU:HD12	1.86	0.41
1:B:657:ARG:CZ	1:B:741:VAL:HG21	2.50	0.40
1:A:470:VAL:CG1	1:A:508:PHE:CD1	3.01	0.40
1:A:398:TRP:HD1	1:A:482:ARG:HH22	1.69	0.40
1:A:521:PHE:O	1:A:525:GLN:HG2	2.21	0.40
1:B:460:ILE:C	1:B:462:PRO:HD3	2.41	0.40
1:B:614:ARG:HG2	1:B:618:TYR:CE2	2.56	0.40
1:A:494:ASP:OD1	1:A:494:ASP:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:LEU:O	1:B:701:LYS:NZ[1_545]	2.07	0.13

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	368/375 (98%)	335 (91%)	26 (7%)	7 (2%)	8 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	368/375 (98%)	331 (90%)	29 (8%)	8 (2%)	6	24
All	All	736/750 (98%)	666 (90%)	55 (8%)	15 (2%)	7	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	TRP
1	B	398	TRP
1	B	696	PRO
1	A	610	GLU
1	A	699	ASP
1	B	487	TYR
1	B	500	PHE
1	B	577	GLN
1	B	582	PRO
1	A	443	PHE
1	A	487	TYR
1	B	397	GLY
1	A	577	GLN
1	A	462	PRO
1	B	760	GLY

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	341/345 (99%)	314 (92%)	27 (8%)	12	34
1	B	341/345 (99%)	314 (92%)	27 (8%)	12	34
All	All	682/690 (99%)	628 (92%)	54 (8%)	12	34

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	394	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	399	ARG
1	A	401	LEU
1	A	413	SER
1	A	422	SER
1	A	450	LEU
1	A	482	ARG
1	A	512	SER
1	A	535	ARG
1	A	558	ILE
1	A	580	GLU
1	A	608	ASP
1	A	610	GLU
1	A	661	ASP
1	A	671	LEU
1	A	681	GLN
1	A	691	SER
1	A	693	THR
1	A	694	LEU
1	A	695	THR
1	A	707	VAL
1	A	711	THR
1	A	716	ARG
1	A	722	HIS
1	A	732	ASP
1	A	734	GLU
1	A	744	THR
1	B	399	ARG
1	B	450	LEU
1	B	485	SER
1	B	501	ASP
1	B	548	ARG
1	B	580	GLU
1	B	600	HIS
1	B	622	LEU
1	B	656	TRP
1	B	659	THR
1	B	660	LYS
1	B	669	LEU
1	B	670	LEU
1	B	681	GLN
1	B	683	GLU
1	B	686	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	691	SER
1	B	693	THR
1	B	697	THR
1	B	707	VAL
1	B	709	ARG
1	B	711	THR
1	B	744	THR
1	B	746	SER
1	B	748	ARG
1	B	754	LEU
1	B	761	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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, 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	370/375 (98%)	0.54	11 (2%) 50 45	75, 107, 142, 169	0
1	B	370/375 (98%)	0.56	9 (2%) 59 56	75, 108, 141, 167	0
All	All	740/750 (98%)	0.55	20 (2%) 54 50	75, 107, 142, 169	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	627	LEU	3.4
1	A	487	TYR	3.1
1	B	487	TYR	2.9
1	A	719	ALA	2.7
1	B	643	ILE	2.7
1	A	648	LEU	2.6
1	B	421	ILE	2.5
1	A	460	ILE	2.4
1	A	723	LYS	2.4
1	B	508	PHE	2.3
1	A	720	THR	2.3
1	B	512	SER	2.3
1	B	686	LEU	2.3
1	A	731	TRP	2.2
1	B	720	THR	2.2
1	B	558	ILE	2.1
1	A	670	LEU	2.1
1	A	508	PHE	2.0
1	A	599	LEU	2.0
1	A	724	ALA	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.