



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:16 AM GMT

PDB ID : 3ODW
Title : Crystal Structure of the Linker-DH/PH domains of p115-RhoGEF
Authors : Chen, Z.; Guo, L.; Sprang, S.R.; Sternweis, P.C.
Deposited on : 2010-08-11
Resolution : 3.20 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 ⓘ](#)) 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

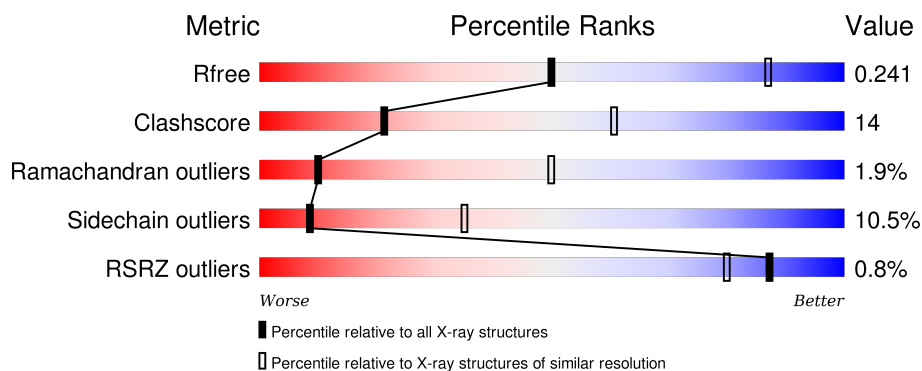
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

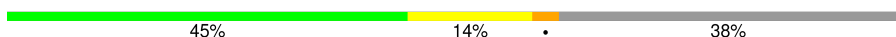
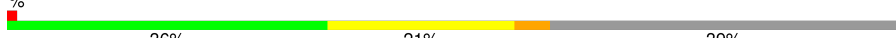
The reported resolution of this entry is 3.20 Å.

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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 $\leq 5\%$. 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	536	 45% 14% • 38%
1	B	536	 36% 21% • 39%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5416 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	331	Total	C	N	O	S	0	0	0
			2729	1730	490	493	16			
1	B	326	Total	C	N	O	S	0	0	0
			2687	1704	483	486	14			

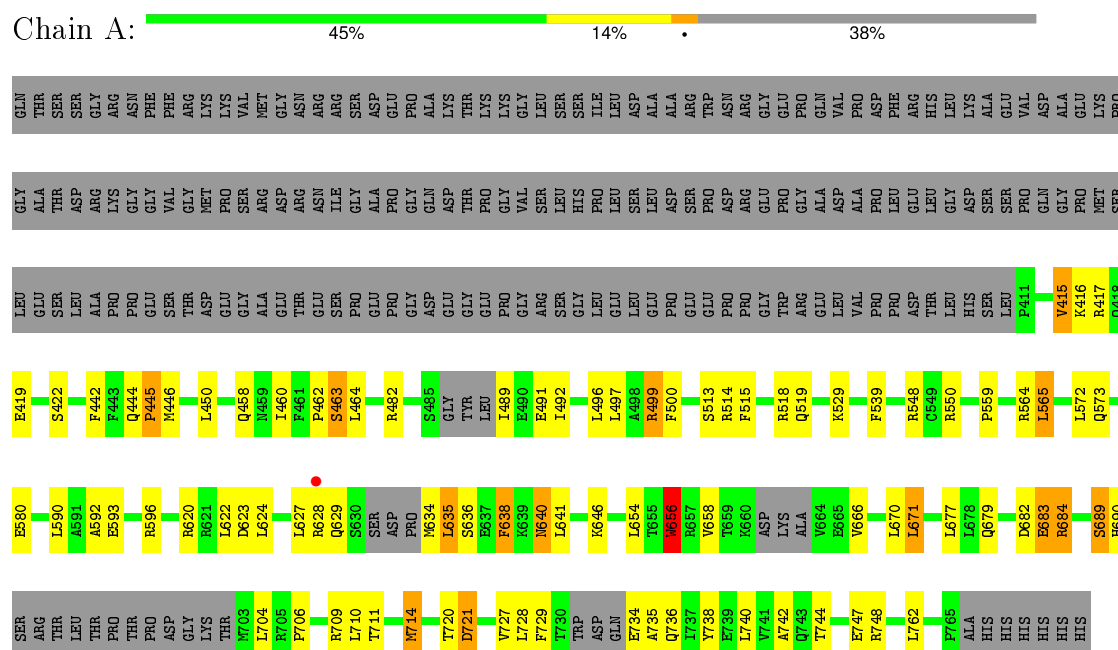
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	GLN	-	EXPRESSION TAG	UNP Q92888
A	238	THR	-	EXPRESSION TAG	UNP Q92888
A	239	SER	-	EXPRESSION TAG	UNP Q92888
A	767	HIS	-	EXPRESSION TAG	UNP Q92888
A	768	HIS	-	EXPRESSION TAG	UNP Q92888
A	769	HIS	-	EXPRESSION TAG	UNP Q92888
A	770	HIS	-	EXPRESSION TAG	UNP Q92888
A	771	HIS	-	EXPRESSION TAG	UNP Q92888
A	772	HIS	-	EXPRESSION TAG	UNP Q92888
B	237	GLN	-	EXPRESSION TAG	UNP Q92888
B	238	THR	-	EXPRESSION TAG	UNP Q92888
B	239	SER	-	EXPRESSION TAG	UNP Q92888
B	767	HIS	-	EXPRESSION TAG	UNP Q92888
B	768	HIS	-	EXPRESSION TAG	UNP Q92888
B	769	HIS	-	EXPRESSION TAG	UNP Q92888
B	770	HIS	-	EXPRESSION TAG	UNP Q92888
B	771	HIS	-	EXPRESSION TAG	UNP Q92888
B	772	HIS	-	EXPRESSION TAG	UNP Q92888

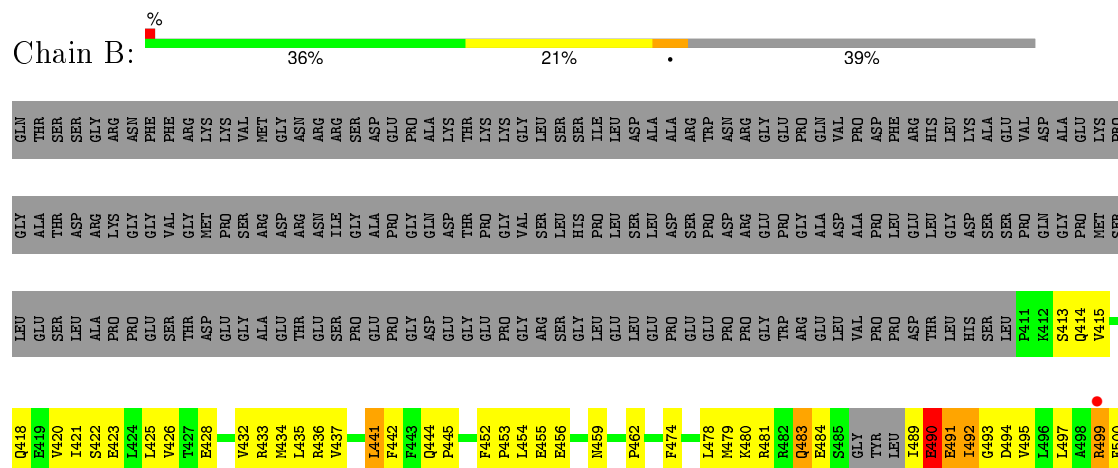
3 Residue-property plots

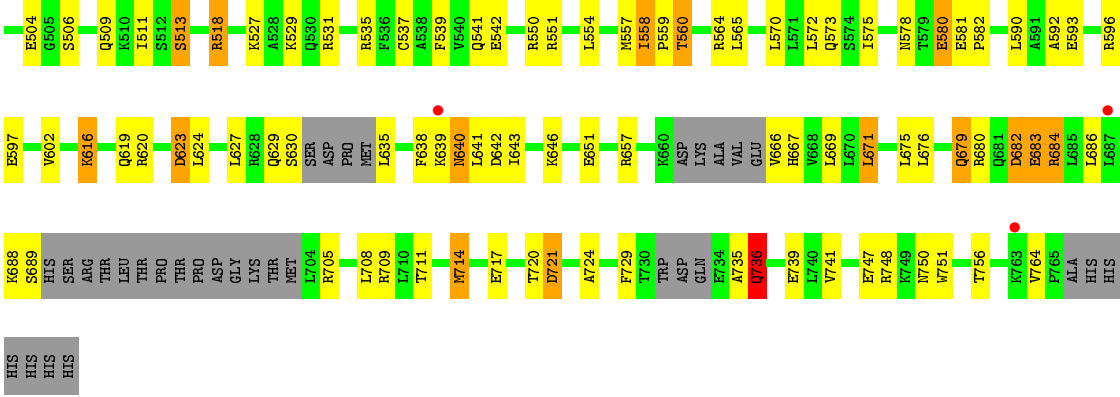
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 1



- Molecule 1: Rho guanine nucleotide exchange factor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	111.64 Å 111.64 Å 97.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.67 – 3.20 43.67 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.67-3.20) 99.5 (43.67-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.231 , 0.289 0.229 , 0.241	Depositor DCC
R_{free} test set	1144 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
Estimated twinning fraction	0.008 for -h,-k,l 0.448 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22445 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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, 0.375 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	0.73	4/2770 (0.1%)	0.84	4/3721 (0.1%)
1	B	0.94	4/2727 (0.1%)	1.05	7/3664 (0.2%)
All	All	0.84	8/5497 (0.1%)	0.95	11/7385 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	684	ARG	CZ-NH1	16.19	1.54	1.33
1	A	684	ARG	CD-NE	13.16	1.68	1.46
1	B	623	ASP	CB-CG	11.23	1.75	1.51
1	A	684	ARG	CZ-NH1	-8.02	1.22	1.33
1	B	684	ARG	CZ-NH2	6.82	1.42	1.33
1	A	623	ASP	CB-CG	6.27	1.65	1.51
1	A	684	ARG	NE-CZ	6.00	1.40	1.33
1	B	490	GLU	CG-CD	5.27	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	684	ARG	NE-CZ-NH1	-31.79	104.41	120.30
1	B	684	ARG	NH1-CZ-NH2	12.23	132.85	119.40
1	A	684	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	A	623	ASP	CB-CG-OD2	-11.42	108.02	118.30
1	A	623	ASP	CB-CG-OD1	10.73	127.96	118.30
1	A	656	TRP	CA-CB-CG	6.07	125.23	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	684	ARG	CD-NE-CZ	5.60	131.44	123.60
1	B	686	LEU	CA-CB-CG	5.51	127.98	115.30
1	B	623	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	623	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	623	ASP	OD1-CG-OD2	-5.08	113.65	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	684	ARG	Sidechain

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	2729	0	2802	66	0
1	B	2687	0	2762	94	1
All	All	5416	0	5564	156	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 14.

All (156) 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:623:ASP:CB	1:B:623:ASP:CG	1.75	1.55
1:A:684:ARG:CD	1:A:684:ARG:NE	1.68	1.54
1:B:717:GLU:HG3	1:B:748:ARG:HH12	1.05	1.19
1:A:634:MET:HE2	1:A:635:LEU:HD12	1.31	1.12
1:B:717:GLU:HG3	1:B:748:ARG:NH1	1.67	1.09
1:B:499:ARG:NH2	1:B:500:PHE:CE2	2.21	1.08
1:A:634:MET:HE2	1:A:635:LEU:CD1	1.83	1.08
1:B:499:ARG:NH2	1:B:500:PHE:CZ	2.26	1.04
1:B:444:GLN:HB3	1:B:445:PRO:HD3	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:HD2	1:A:489:ILE:HD11	1.41	1.00
1:B:735:ALA:HA	1:B:736:GLN:HB2	1.46	0.96
1:B:557:MET:O	1:B:560:THR:HB	1.71	0.90
1:A:634:MET:CE	1:A:635:LEU:CD1	2.52	0.88
1:B:481:ARG:HA	1:B:484:GLU:OE2	1.75	0.86
1:A:711:THR:HG22	1:A:762:LEU:HD23	1.58	0.86
1:A:735:ALA:HA	1:A:736:GLN:HB2	1.58	0.83
1:A:728:LEU:HD11	1:B:425:LEU:HD21	1.61	0.81
1:A:634:MET:HE2	1:A:635:LEU:CG	2.12	0.80
1:B:527:LYS:HD2	1:B:531:ARG:HH21	1.47	0.79
1:B:565:LEU:HD21	1:B:602:VAL:HG21	1.64	0.79
1:A:720:THR:O	1:A:721:ASP:HB2	1.83	0.79
1:B:735:ALA:CA	1:B:736:GLN:HB2	2.13	0.78
1:B:573:GLN:HE21	1:B:596:ARG:HH11	1.31	0.77
1:B:420:VAL:HG12	1:B:575:ILE:HG13	1.67	0.76
1:A:734:GLU:HA	1:A:734:GLU:OE1	1.84	0.76
1:A:656:TRP:CH2	1:A:704:LEU:HD13	2.22	0.75
1:A:634:MET:CE	1:A:635:LEU:HD12	2.11	0.75
1:A:656:TRP:HH2	1:A:704:LEU:HD13	1.51	0.74
1:A:735:ALA:H	1:A:736:GLN:HG2	1.55	0.71
1:A:634:MET:CE	1:A:635:LEU:HG	2.21	0.71
1:B:490:GLU:O	1:B:491:GLU:HB3	1.91	0.70
1:B:444:GLN:HB3	1:B:445:PRO:CD	2.20	0.69
1:B:565:LEU:CD2	1:B:602:VAL:HG21	2.24	0.68
1:B:420:VAL:CG1	1:B:575:ILE:HG13	2.22	0.67
1:B:499:ARG:NH1	1:B:500:PHE:CE1	2.63	0.67
1:A:499:ARG:NH2	1:A:500:PHE:CE2	2.54	0.67
1:B:437:VAL:HG13	1:B:441:LEU:HD22	1.76	0.65
1:A:683:GLU:HG2	1:A:684:ARG:N	2.13	0.63
1:B:474:PHE:HB2	1:B:499:ARG:HD3	1.79	0.63
1:A:638:PHE:HB3	1:A:641:LEU:HB2	1.81	0.62
1:B:572:LEU:N	1:B:572:LEU:HD12	2.15	0.61
1:A:442:PHE:O	1:A:446:MET:HG3	2.00	0.61
1:B:682:ASP:CG	1:B:683:GLU:H	2.04	0.61
1:A:519:GLN:NE2	1:A:559:PRO:HB3	2.16	0.61
1:B:724:ALA:HB2	1:B:741:VAL:HG22	1.82	0.61
1:A:499:ARG:NH1	1:A:500:PHE:CE1	2.61	0.60
1:B:453:PRO:HB2	1:B:455:GLU:OE1	2.02	0.60
1:A:689:SER:HA	1:A:706:PRO:HD3	1.82	0.59
1:B:432:VAL:O	1:B:436:ARG:HG3	2.01	0.58
1:B:638:PHE:HB3	1:B:641:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:VAL:HG12	1:B:679:GLN:HG3	1.84	0.58
1:A:658:VAL:HG21	1:A:690:HIS:HD1	1.65	0.58
1:B:669:LEU:HB3	1:B:671:LEU:HD13	1.85	0.58
1:B:518:ARG:HH11	1:B:518:ARG:HG2	1.69	0.58
1:A:634:MET:HE3	1:A:635:LEU:HG	1.85	0.57
1:B:420:VAL:HG12	1:B:575:ILE:CG1	2.35	0.57
1:B:483:GLN:HA	1:B:483:GLN:OE1	2.05	0.56
1:A:735:ALA:N	1:A:736:GLN:HG2	2.21	0.56
1:B:590:LEU:O	1:B:593:GLU:HB3	2.05	0.56
1:B:489:ILE:HG23	1:B:490:GLU:N	2.22	0.55
1:A:462:PRO:HG2	1:A:518:ARG:HB2	1.89	0.55
1:B:499:ARG:CZ	1:B:500:PHE:CZ	2.89	0.54
1:A:735:ALA:CA	1:A:736:GLN:HB2	2.34	0.54
1:A:573:GLN:HE21	1:A:596:ARG:HH11	1.54	0.54
1:A:684:ARG:CG	1:A:684:ARG:NE	2.65	0.53
1:A:634:MET:O	1:A:636:SER:N	2.34	0.53
1:B:669:LEU:HB2	1:B:676:LEU:HB2	1.91	0.53
1:B:651:GLU:OE1	1:B:667:HIS:HE1	1.91	0.52
1:A:572:LEU:HB3	1:A:592:ALA:HB2	1.92	0.52
1:B:708:LEU:HD22	1:B:729:PHE:CE2	2.45	0.52
1:B:580:GLU:CD	1:B:581:GLU:H	2.13	0.52
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.91	0.52
1:A:714:MET:HE1	1:B:433:ARG:HB2	1.91	0.52
1:B:629:GLN:O	1:B:630:SER:C	2.48	0.52
1:A:684:ARG:CZ	1:A:684:ARG:CD	2.77	0.51
1:A:735:ALA:HB2	1:B:426:VAL:HG23	1.91	0.51
1:A:646:LYS:HE3	1:A:671:LEU:HD23	1.92	0.51
1:A:634:MET:CE	1:A:635:LEU:CG	2.77	0.51
1:B:421:ILE:HG12	1:B:492:ILE:HD13	1.93	0.51
1:B:639:LYS:HB3	1:B:640:ASN:HB3	1.91	0.51
1:B:478:LEU:HD23	1:B:495:VAL:HG11	1.93	0.51
1:B:735:ALA:CA	1:B:736:GLN:CB	2.88	0.50
1:B:572:LEU:CD1	1:B:572:LEU:N	2.75	0.49
1:A:638:PHE:CB	1:A:641:LEU:HB2	2.41	0.49
1:B:454:LEU:O	1:B:455:GLU:C	2.51	0.49
1:B:635:LEU:HD21	1:B:705:ARG:HD2	1.95	0.49
1:B:616:LYS:HE2	1:B:620:ARG:NH1	2.28	0.49
1:B:747:GLU:O	1:B:751:TRP:HD1	1.96	0.48
1:A:656:TRP:HB2	1:A:740:LEU:HD23	1.95	0.47
1:A:738:TYR:N	1:A:738:TYR:CD2	2.81	0.47
1:B:445:PRO:HB2	1:B:539:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ASP:CG	1:B:623:ASP:CA	2.74	0.47
1:A:720:THR:O	1:A:721:ASP:CB	2.60	0.47
1:B:490:GLU:O	1:B:491:GLU:CB	2.61	0.47
1:B:593:GLU:O	1:B:597:GLU:HG3	2.15	0.47
1:A:445:PRO:HB2	1:A:539:PHE:HZ	1.80	0.47
1:B:537:CYS:O	1:B:541:GLN:HG3	2.14	0.47
1:B:418:GLN:HE22	1:B:489:ILE:HB	1.79	0.47
1:A:415:VAL:O	1:A:419:GLU:HG3	2.15	0.47
1:A:580:GLU:N	1:A:580:GLU:OE1	2.44	0.47
1:A:690:HIS:ND1	1:A:690:HIS:O	2.48	0.46
1:B:714:MET:HE2	1:B:714:MET:HB2	1.63	0.46
1:A:492:ILE:O	1:A:492:ILE:HG12	2.14	0.46
1:B:499:ARG:NH1	1:B:500:PHE:CZ	2.83	0.46
1:A:727:VAL:HG12	1:A:729:PHE:CE2	2.51	0.46
1:A:499:ARG:NH1	1:A:500:PHE:CZ	2.78	0.46
1:B:572:LEU:HB3	1:B:592:ALA:HB2	1.97	0.46
1:B:442:PHE:CD1	1:B:554:LEU:HD13	2.51	0.46
1:A:463:SER:O	1:A:464:LEU:C	2.52	0.46
1:A:590:LEU:O	1:A:593:GLU:HB3	2.16	0.46
1:B:489:ILE:HG23	1:B:490:GLU:H	1.81	0.46
1:B:558:ILE:N	1:B:559:PRO:CD	2.79	0.45
1:B:413:SER:HA	1:B:578:ASN:OD1	2.16	0.45
1:B:428:GLU:OE1	1:B:564:ARG:NH2	2.47	0.45
1:A:496:LEU:HG	1:A:572:LEU:HD21	1.99	0.45
1:B:735:ALA:N	1:B:736:GLN:HB2	2.32	0.45
1:A:654:LEU:HD12	1:A:742:ALA:HA	1.99	0.45
1:A:462:PRO:HB2	1:A:515:PHE:HA	1.99	0.45
1:A:460:ILE:C	1:A:462:PRO:HD3	2.37	0.44
1:B:643:ILE:HA	1:B:646:LYS:HD2	1.99	0.44
1:B:581:GLU:HA	1:B:582:PRO:HD2	1.81	0.44
1:A:499:ARG:NH2	1:A:500:PHE:CD2	2.85	0.44
1:A:735:ALA:CA	1:A:736:GLN:CB	2.96	0.43
1:B:493:GLY:O	1:B:497:LEU:HD12	2.18	0.43
1:B:669:LEU:O	1:B:675:LEU:HD12	2.17	0.43
1:B:422:SER:O	1:B:423:GLU:C	2.56	0.43
1:A:670:LEU:HD11	1:A:710:LEU:HD11	2.01	0.43
1:B:459:ASN:HB2	1:B:518:ARG:HD3	2.00	0.43
1:B:682:ASP:CG	1:B:683:GLU:N	2.69	0.43
1:B:479:MET:O	1:B:480:LYS:C	2.57	0.43
1:A:735:ALA:HB1	1:B:425:LEU:HD22	2.01	0.42
1:B:425:LEU:HD23	1:B:425:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:LEU:HD13	1:B:671:LEU:HD11	2.01	0.42
1:B:414:GLN:O	1:B:415:VAL:C	2.58	0.42
1:A:627:LEU:C	1:A:629:GLN:H	2.21	0.42
1:A:564:ARG:HD2	1:A:564:ARG:HA	1.78	0.42
1:B:509:GLN:O	1:B:513:SER:HB3	2.19	0.42
1:A:670:LEU:CD1	1:A:710:LEU:HD11	2.50	0.42
1:B:657:ARG:HD3	1:B:739:GLU:OE2	2.20	0.42
1:B:441:LEU:N	1:B:441:LEU:CD1	2.82	0.42
1:B:669:LEU:HB3	1:B:671:LEU:CD1	2.48	0.41
1:B:435:LEU:HA	1:B:435:LEU:HD23	1.76	0.41
1:B:747:GLU:HA	1:B:750:ASN:HB3	2.01	0.41
1:B:627:LEU:HD23	1:B:638:PHE:HB2	2.03	0.41
1:A:744:THR:HG23	1:A:747:GLU:H	1.85	0.41
1:B:494:ASP:OD1	1:B:494:ASP:N	2.53	0.41
1:B:639:LYS:HB3	1:B:640:ASN:CB	2.51	0.41
1:B:720:THR:O	1:B:721:ASP:HB2	2.20	0.41
1:A:463:SER:OG	1:A:514:ARG:NH1	2.54	0.41
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.64	0.41
1:B:619:GLN:OE1	1:B:642:ASP:HA	2.20	0.41
1:B:474:PHE:CZ	1:B:499:ARG:NH2	2.88	0.41
1:A:734:GLU:CA	1:A:734:GLU:OE1	2.59	0.40
1:B:418:GLN:OE1	1:B:418:GLN:HA	2.21	0.40
1:B:462:PRO:HG2	1:B:518:ARG:HB2	2.04	0.40
1:B:511:ILE:HD13	1:B:511:ILE:HA	1.68	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:B:504:GLU:OE1	1:B:535:ARG:NH1[2_654]	2.18	0.02

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	319/536 (60%)	285 (89%)	27 (8%)	7 (2%)	8	45
1	B	314/536 (59%)	265 (84%)	44 (14%)	5 (2%)	12	54
All	All	633/1072 (59%)	550 (87%)	71 (11%)	12 (2%)	10	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	LEU
1	A	721	ASP
1	B	490	GLU
1	B	721	ASP
1	A	565	LEU
1	B	492	ILE
1	B	736	GLN
1	A	640	ASN
1	B	491	GLU
1	A	682	ASP
1	A	548	ARG
1	A	491	GLU

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	306/476 (64%)	276 (90%)	30 (10%)	10	38
1	B	301/476 (63%)	267 (89%)	34 (11%)	7	31
All	All	607/952 (64%)	543 (90%)	64 (10%)	8	35

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	VAL
1	A	416	LYS

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Mol	Chain	Res	Type
1	A	417	ARG
1	A	422	SER
1	A	445	PRO
1	A	450	LEU
1	A	458	GLN
1	A	463	SER
1	A	497	LEU
1	A	499	ARG
1	A	513	SER
1	A	529	LYS
1	A	550	ARG
1	A	565	LEU
1	A	620	ARG
1	A	622	LEU
1	A	624	LEU
1	A	628	ARG
1	A	638	PHE
1	A	640	ASN
1	A	656	TRP
1	A	666	VAL
1	A	671	LEU
1	A	677	LEU
1	A	679	GLN
1	A	683	GLU
1	A	689	SER
1	A	709	ARG
1	A	714	MET
1	A	748	ARG
1	B	434	MET
1	B	441	LEU
1	B	452	PHE
1	B	456	GLU
1	B	483	GLN
1	B	490	GLU
1	B	499	ARG
1	B	506	SER
1	B	513	SER
1	B	518	ARG
1	B	529	LYS
1	B	542	GLU
1	B	550	ARG
1	B	551	ARG

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Mol	Chain	Res	Type
1	B	558	ILE
1	B	560	THR
1	B	570	LEU
1	B	580	GLU
1	B	616	LYS
1	B	624	LEU
1	B	640	ASN
1	B	671	LEU
1	B	679	GLN
1	B	680	ARG
1	B	682	ASP
1	B	683	GLU
1	B	688	LYS
1	B	689	SER
1	B	709	ARG
1	B	711	THR
1	B	714	MET
1	B	736	GLN
1	B	756	THR
1	B	764	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	573	GLN
1	A	681	GLN
1	B	414	GLN
1	B	509	GLN
1	B	573	GLN
1	B	604	GLN
1	B	667	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 [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 [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	331/536 (61%)	0.00	1 (0%) 94 93	53, 85, 140, 199	0
1	B	326/536 (60%)	0.04	4 (1%) 81 69	62, 98, 145, 202	0
All	All	657/1072 (61%)	0.02	5 (0%) 87 80	53, 95, 143, 202	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	763	LYS	2.9
1	B	639	LYS	2.6
1	B	687	LEU	2.4
1	A	628	ARG	2.4
1	B	499	ARG	2.2

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.