



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:36 PM UTC

PDB ID : 3ODW / pdb_00003odw
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

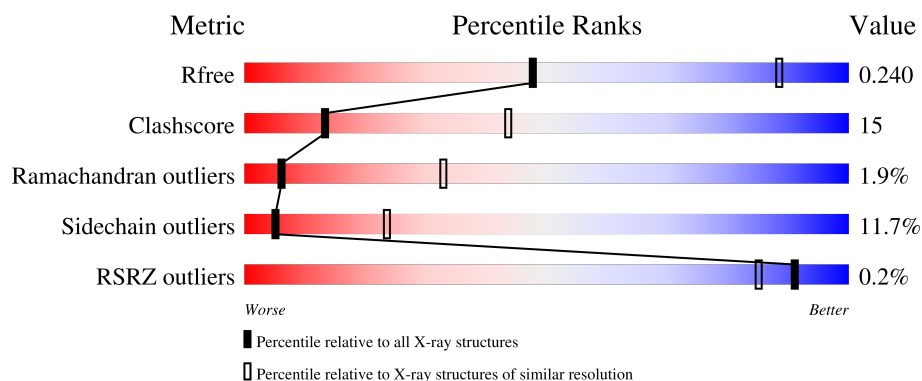
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

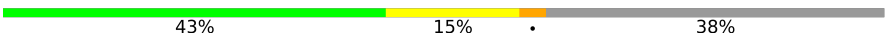
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	
1	B	536	

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			

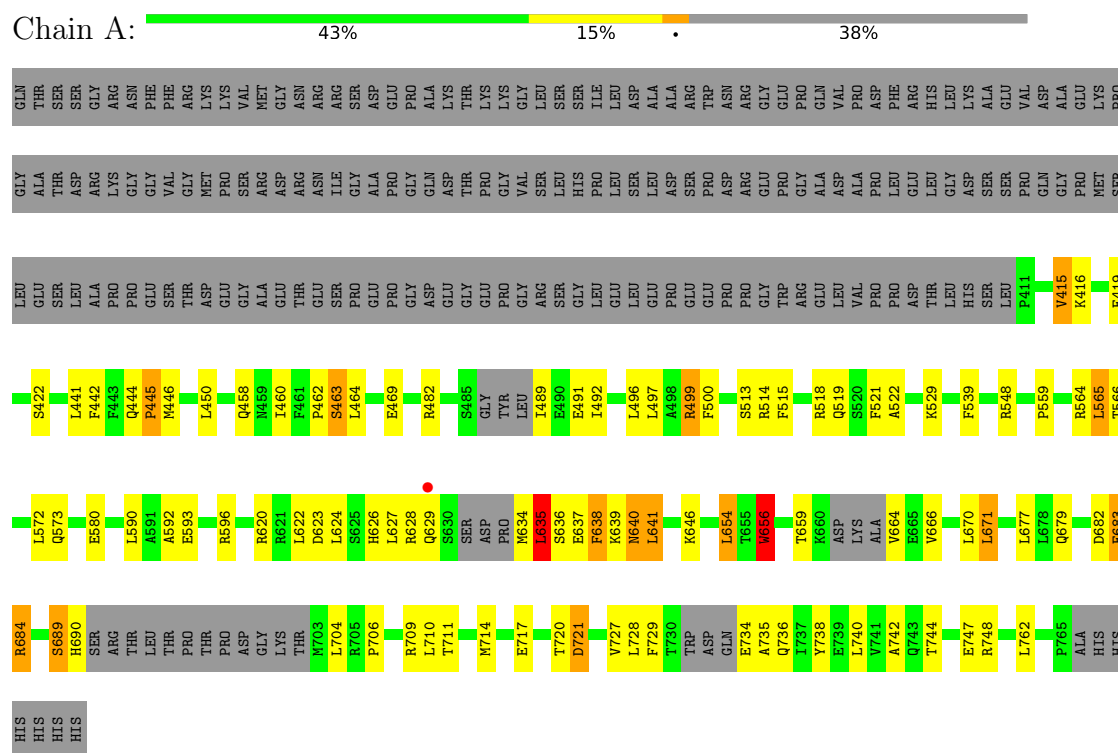
There are 18 discrepancies between the modelled and reference sequences:

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

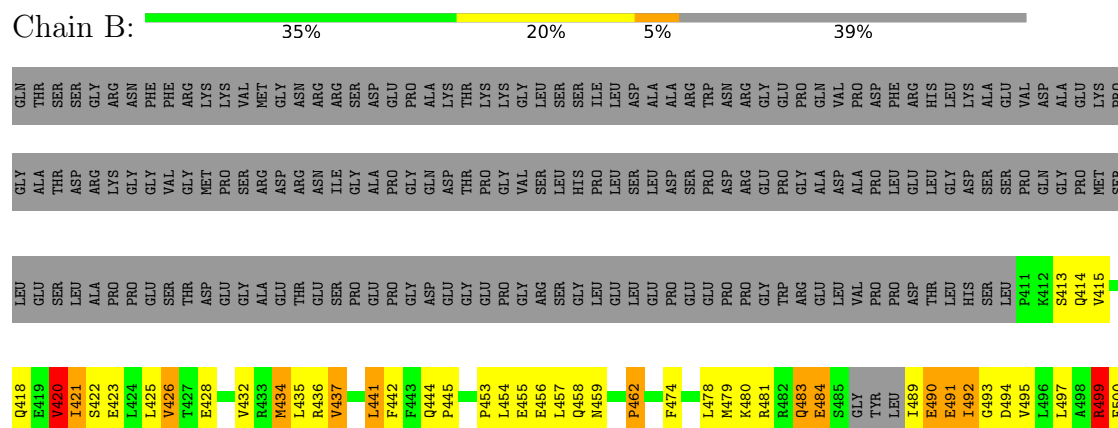
3 Residue-property plots

These plots are drawn for all protein, RNA, 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



- 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	111.64Å 111.64Å 97.88Å 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 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.231 , 0.289 0.229 , 0.240	Depositor DCC
R_{free} test set	1147 reflections (5.11%)	wwPDB-VP
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 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.448 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	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, 0.333 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	0.93	6/2770 (0.2%)	1.07	8/3721 (0.2%)
1	B	1.02	3/2727 (0.1%)	1.21	14/3664 (0.4%)
All	All	0.97	9/5497 (0.2%)	1.14	22/7385 (0.3%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	684	ARG	CD-NE	16.12	1.68	1.46
1	B	684	ARG	CZ-NH1	15.25	1.54	1.32
1	B	623	ASP	CB-CG	9.31	1.75	1.52
1	A	684	ARG	CZ-NH1	-7.24	1.22	1.32
1	A	684	ARG	NE-CZ	7.09	1.40	1.33
1	A	659	THR	CA-CB	6.67	1.62	1.53
1	B	684	ARG	CZ-NH2	6.51	1.42	1.33
1	A	626	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	623	ASP	CB-CG	5.14	1.65	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	684	ARG	NE-CZ-NH1	-17.09	104.41	121.50
1	B	684	ARG	NH1-CZ-NH2	10.42	132.85	119.30
1	A	684	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	B	658	VAL	N-CA-C	-7.34	105.49	111.81
1	B	462	PRO	CA-C-N	-7.04	111.14	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	462	PRO	C-N-CA	-7.04	111.14	122.62
1	B	639	LYS	N-CA-C	6.35	119.15	111.40
1	A	656	TRP	CA-CB-CG	6.12	125.23	113.60
1	B	639	LYS	CA-C-N	6.06	132.60	121.70
1	B	639	LYS	C-N-CA	6.06	132.60	121.70
1	B	458	GLN	CA-C-N	-5.76	113.44	122.65
1	B	458	GLN	C-N-CA	-5.76	113.44	122.65
1	A	635	LEU	N-CA-C	5.72	122.98	110.80
1	A	639	LYS	CA-C-N	5.67	131.91	121.70
1	A	639	LYS	C-N-CA	5.67	131.91	121.70
1	A	469	GLU	N-CA-C	5.54	117.32	111.28
1	B	437	VAL	CB-CA-C	-5.48	104.96	111.97
1	B	499	ARG	N-CA-C	5.48	120.06	112.45
1	A	639	LYS	N-CA-C	5.41	119.88	113.12
1	A	626	HIS	CE1-NE2-CD2	5.25	114.25	109.00
1	B	420	VAL	N-CA-C	5.21	115.35	110.30
1	B	684	ARG	CD-NE-CZ	5.03	131.44	124.40

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	67	0
1	B	2687	0	2762	98	1
All	All	5416	0	5564	162	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 15.

All (162) 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	1.59
1:A:684:ARG:NE	1:A:684:ARG:CD	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	1.22	1.15
1:B:717:GLU:HG3	1:B:748:ARG:NH1	1.67	1.09
1:A:634:MET:HE2	1:A:635:LEU:CD1	1.81	1.09
1:B:499:ARG:NH2	1:B:500:PHE:CE2	2.21	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
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:B:527:LYS:HD2	1:B:531:ARG:HH21	1.47	0.79
1:A:720:THR:O	1:A:721:ASP:HB2	1.83	0.79
1:B:565:LEU:HD21	1:B:602:VAL:HG21	1.64	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:656:TRP:HH2	1:A:704:LEU:HD13	1.51	0.74
1:A:634:MET:HE3	1:A:635:LEU:HG	1.68	0.74
1:A:634:MET:CE	1:A:635:LEU:HD12	2.11	0.73
1:A:735:ALA:H	1:A:736:GLN:HG2	1.55	0.71
1:B:490:GLU:O	1:B:491:GLU:HB3	1.91	0.70
1:A:634:MET:CE	1:A:635:LEU:HG	2.21	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:A:634:MET:HE2	1:A:635:LEU:CG	2.24	0.67
1:B:420:VAL:CG1	1:B:575:ILE:HG13	2.22	0.67
1:A:499:ARG:NH2	1:A:500:PHE:CE2	2.54	0.67
1:B:499:ARG:NH1	1:B:500:PHE:CE1	2.63	0.67
1:B:437:VAL:HG13	1:B:441:LEU:HD22	1.76	0.65
1:B:682:ASP:CG	1:B:683:GLU:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:PHE:O	1:A:446:MET:HG3	2.00	0.61
1:B:572:LEU:HD12	1:B:572:LEU:N	2.15	0.61
1:A:634:MET:CE	1:A:635:LEU:CG	2.77	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
1:B:666:VAL:HG12	1:B:679:GLN:HG3	1.84	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: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:B:580:GLU:CD	1:B:581:GLU:H	2.13	0.56
1:B:629:GLN:O	1:B:630:SER:C	2.48	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:A:735:ALA:CA	1:A:736:GLN:HB2	2.34	0.54
1:B:499:ARG:CZ	1:B:500:PHE:CZ	2.89	0.54
1:A:573:GLN:HE21	1:A:596:ARG:HH11	1.54	0.54
1:B:454:LEU:O	1:B:455:GLU:C	2.51	0.54
1:A:684:ARG:NE	1:A:684:ARG:CG	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:A:444:GLN:HB3	1:A:445:PRO:HD3	1.91	0.52
1:A:646:LYS:HE3	1:A:671:LEU:HD23	1.92	0.51
1:A:684:ARG:CD	1:A:684:ARG:CZ	2.77	0.51
1:A:735:ALA:HB2	1:B:426:VAL:HG23	1.91	0.51
1:B:623:ASP:CG	1:B:623:ASP:CA	2.74	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:A:463:SER:O	1:A:464:LEU:C	2.52	0.50
1:B:735:ALA:CA	1:B:736:GLN:CB	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:MET:HE2	1:B:560:THR:HG21	1.92	0.50
1:B:572:LEU:N	1:B:572:LEU:CD1	2.75	0.49
1:A:638:PHE:CB	1:A:641:LEU:HB2	2.41	0.49
1:A:460:ILE:C	1:A:462:PRO:HD3	2.37	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:B:479:MET:O	1:B:480:LYS:C	2.57	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
1:B:682:ASP:CG	1:B:683:GLU:N	2.69	0.47
1:B:414:GLN:O	1:B:415:VAL:C	2.58	0.47
1:B:425:LEU:C	1:B:425:LEU:HD23	2.40	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:A:627:LEU:C	1:A:629:GLN:H	2.21	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:B:422:SER:O	1:B:423:GLU:C	2.56	0.47
1:A:415:VAL:O	1:A:419:GLU:HG3	2.15	0.47
1:A:580:GLU:OE1	1:A:580:GLU:N	2.44	0.47
1:A:492:ILE:O	1:A:492:ILE:HG12	2.14	0.46
1:A:690:HIS:ND1	1:A:690:HIS:O	2.48	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:442:PHE:CD1	1:B:554:LEU:HD13	2.51	0.46
1:B:572:LEU:HB3	1:B:592:ALA:HB2	1.97	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:B:455:GLU:H	1:B:455:GLU:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:VAL:HG11	1:A:690:HIS:HE2	1.82	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: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:714:MET:HB2	1:B:714:MET:HE2	1.39	0.43
1:A:735:ALA:HB1	1:B:425:LEU:HD22	2.01	0.42
1:A:564:ARG:HA	1:A:564:ARG:HD2	1.78	0.42
1:B:669:LEU:HD13	1:B:671:LEU:HD11	2.01	0.42
1:B:509:GLN:O	1:B:513:SER:HB3	2.19	0.42
1:B:562:MET:HE1	1:B:606:VAL:HG21	2.02	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:435:LEU:HA	1:B:435:LEU:HD23	1.76	0.41
1:B:669:LEU:HB3	1:B:671:LEU:CD1	2.48	0.41
1:B:747:GLU:HA	1:B:750:ASN:HB3	2.01	0.41
1:A:744:THR:HG23	1:A:747:GLU:H	1.85	0.41
1:B:494:ASP:N	1:B:494:ASP:OD1	2.53	0.41
1:B:627:LEU:HD23	1:B:638:PHE:HB2	2.03	0.41
1:B:420:VAL:O	1:B:421:ILE:C	2.64	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:HA	1:A:464:LEU:HD12	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:B:627:LEU:C	1:B:629:GLN:H	2.28	0.41
1:A:635:LEU:C	1:A:637:GLU:H	2.28	0.40
1:A:734:GLU:OE1	1:A:734:GLU:CA	2.59	0.40
1:B:462:PRO:HG2	1:B:518:ARG:HB2	2.04	0.40
1:B:549:CYS:SG	1:B:557:MET:HE1	2.62	0.40
1:A:521:PHE:O	1:A:522:ALA:C	2.65	0.40
1:B:511:ILE:HA	1:B:511:ILE:HD13	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%)	5	29
1	B	314/536 (59%)	265 (84%)	44 (14%)	5 (2%)	7	36
All	All	633/1072 (59%)	550 (87%)	71 (11%)	12 (2%)	6	33

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 [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	306/476 (64%)	273 (89%)	33 (11%)	6	27
1	B	301/476 (63%)	263 (87%)	38 (13%)	4	21
All	All	607/952 (64%)	536 (88%)	71 (12%)	5	23

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	VAL
1	A	416	LYS
1	A	422	SER
1	A	441	LEU
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	565	LEU
1	A	566	THR
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	641	LEU
1	A	654	LEU
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	717	GLU
1	A	748	ARG
1	B	420	VAL

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Mol	Chain	Res	Type
1	B	421	ILE
1	B	426	VAL
1	B	434	MET
1	B	441	LEU
1	B	456	GLU
1	B	457	LEU
1	B	483	GLN
1	B	484	GLU
1	B	499	ARG
1	B	506	SER
1	B	513	SER
1	B	514	ARG
1	B	518	ARG
1	B	529	LYS
1	B	550	ARG
1	B	558	ILE
1	B	560	THR
1	B	570	LEU
1	B	580	GLU
1	B	587	LYS
1	B	616	LYS
1	B	622	LEU
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	707	VAL
1	B	709	ARG
1	B	711	THR
1	B	714	MET
1	B	756	THR
1	B	764	VAL

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

Mol	Chain	Res	Type
1	A	573	GLN

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Mol	Chain	Res	Type
1	A	578	ASN
1	A	650	HIS
1	B	414	GLN
1	B	525	GLN
1	B	573	GLN
1	B	604	GLN
1	B	667	HIS

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 oligosaccharides 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%)	-0.93	1 (0%) 90 81	53, 85, 140, 199	0
1	B	326/536 (60%)	-0.92	0 100 100	62, 98, 145, 202	0
All	All	657/1072 (61%)	-0.92	1 (0%) 91 85	53, 95, 143, 202	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	GLN	2.3

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 oligosaccharides 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.