



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:09 am GMT

PDB ID : 3ODX
Title : Crystal Structure of an N-terminally Truncated Linker-DH/PH Domains of p115-RhoGEF
Authors : Chen, Z.; Guo, L.; Sprang, S.R.; Sternweis, P.C.
Deposited on : 2010-08-12
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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

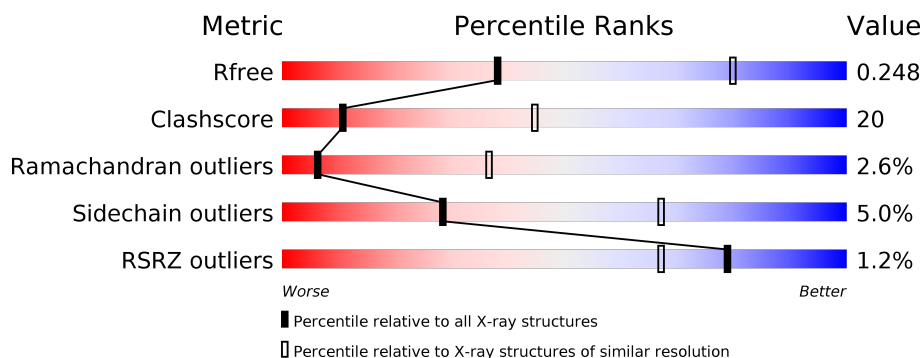
1 Overall quality at a glance ⓘ

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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	417	<div> <div></div> <div> <div></div> <div>50%</div> <div>27%</div> <div>• •</div> <div>19%</div> </div> </div>
1	B	417	<div> <div></div> <div> <div></div> <div>52%</div> <div>24%</div> <div>• •</div> <div>20%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5516 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	336	Total	C	N	O	S	0	0	0
			2762	1748	496	504	14			
1	B	335	Total	C	N	O	S	0	0	0
			2754	1744	493	502	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	GLN	-	EXPRESSION TAG	UNP Q92888
A	351	THR	-	EXPRESSION TAG	UNP Q92888
A	352	SER	-	EXPRESSION TAG	UNP Q92888
B	350	GLN	-	EXPRESSION TAG	UNP Q92888
B	351	THR	-	EXPRESSION TAG	UNP Q92888
B	352	SER	-	EXPRESSION TAG	UNP Q92888

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	111.50Å 111.50Å 97.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.90 – 3.20 48.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.90-3.20) 99.9 (48.89-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.225 , 0.274 0.227 , 0.248	Depositor DCC
R_{free} test set	1143 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l 0.478 for h,-h-k,-l 0.010 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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	0.81	4/2805 (0.1%)	0.82	5/3772 (0.1%)
1	B	1.22	12/2797 (0.4%)	1.24	16/3762 (0.4%)
All	All	1.03	16/5602 (0.3%)	1.05	21/7534 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	689	SER	C-O	25.31	1.71	1.23
1	B	684	ARG	CZ-NH1	24.33	1.64	1.33
1	B	689	SER	CB-OG	17.50	1.65	1.42
1	A	628	ARG	CZ-NH1	10.74	1.47	1.33
1	B	684	ARG	NE-CZ	10.42	1.46	1.33
1	B	621	ARG	CZ-NH2	10.05	1.46	1.33
1	B	656	TRP	CE3-CZ3	9.17	1.54	1.38
1	B	656	TRP	NE1-CE2	9.17	1.49	1.37
1	B	623	ASP	CB-CG	8.74	1.70	1.51
1	B	656	TRP	CD2-CE3	7.83	1.52	1.40
1	A	631	SER	CB-OG	6.38	1.50	1.42
1	B	507	TRP	CB-CG	5.55	1.60	1.50
1	B	631	SER	CB-OG	5.27	1.49	1.42
1	B	656	TRP	CG-CD1	5.27	1.44	1.36
1	A	578	ASN	C-N	5.24	1.46	1.34
1	A	507	TRP	CB-CG	5.08	1.59	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	621	ARG	NE-CZ-NH1	-27.97	106.31	120.30
1	B	684	ARG	NE-CZ-NH1	26.46	133.53	120.30
1	B	621	ARG	NE-CZ-NH2	26.01	133.30	120.30
1	B	623	ASP	CB-CG-OD2	16.93	133.54	118.30
1	B	621	ARG	CD-NE-CZ	10.64	138.49	123.60
1	B	684	ARG	NH1-CZ-NH2	-10.41	107.94	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	656	TRP	CH2-CZ2-CE2	7.72	125.12	117.40
1	B	623	ASP	OD1-CG-OD2	-7.28	109.47	123.30
1	B	656	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	B	656	TRP	CG-CD2-CE3	6.45	139.70	133.90
1	A	499	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	656	TRP	CD1-CG-CD2	6.37	111.39	106.30
1	A	518	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	628	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	748	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	656	TRP	CE3-CZ3-CH2	-5.53	115.11	121.20
1	B	499	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	462	PRO	C-N-CA	-5.32	108.41	121.70
1	A	656	TRP	CA-CB-CG	5.27	123.72	113.70
1	B	585	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	686	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2762	0	2828	118	0
1	B	2754	0	2826	112	0
All	All	5516	0	5654	228	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 20.

All (228) 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:499:ARG:NH2	1:B:500:PHE:CZ	1.78	1.51
1:B:735:ALA:CA	1:B:736:GLN:HB2	1.43	1.46
1:B:689:SER:OG	1:B:689:SER:CB	1.65	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ALA:CA	1:A:736:GLN:HB2	1.46	1.44
1:A:499:ARG:NH2	1:A:500:PHE:CE2	1.85	1.44
1:B:735:ALA:HA	1:B:736:GLN:CB	1.43	1.43
1:B:499:ARG:NH2	1:B:500:PHE:CE2	1.88	1.39
1:A:499:ARG:NH2	1:A:500:PHE:CZ	1.93	1.35
1:B:499:ARG:CZ	1:B:500:PHE:CZ	2.13	1.30
1:A:653:PRO:O	1:A:654:LEU:HD12	1.32	1.28
1:B:689:SER:C	1:B:689:SER:O	1.71	1.28
1:A:735:ALA:HA	1:A:736:GLN:CB	1.68	1.18
1:A:451:PHE:HE1	1:A:535:ARG:HD3	1.12	1.13
1:B:499:ARG:NH1	1:B:500:PHE:CZ	2.18	1.10
1:A:451:PHE:CE1	1:A:535:ARG:HD3	1.92	1.04
1:A:499:ARG:CZ	1:A:500:PHE:CZ	2.40	1.03
1:B:736:GLN:OE1	1:B:736:GLN:HA	1.51	1.02
1:B:499:ARG:CZ	1:B:500:PHE:CE2	2.41	0.99
1:B:489:ILE:HG23	1:B:490:GLU:H	1.27	0.99
1:A:735:ALA:CA	1:A:736:GLN:CB	2.30	0.97
1:A:499:ARG:HH22	1:A:500:PHE:HZ	1.06	0.91
1:A:499:ARG:NH1	1:A:500:PHE:CZ	2.38	0.91
1:B:499:ARG:NH1	1:B:500:PHE:CE1	2.39	0.90
1:A:735:ALA:N	1:A:736:GLN:HB2	1.86	0.89
1:B:717:GLU:HG3	1:B:748:ARG:NH1	1.89	0.88
1:A:499:ARG:NH2	1:A:500:PHE:HE2	1.68	0.87
1:B:444:GLN:HB3	1:B:445:PRO:HD3	1.58	0.85
1:B:717:GLU:HG3	1:B:748:ARG:HH12	1.41	0.85
1:A:735:ALA:N	1:A:736:GLN:HG2	1.91	0.85
1:B:499:ARG:NH2	1:B:500:PHE:HE2	1.67	0.84
1:A:499:ARG:CZ	1:A:500:PHE:CE2	2.60	0.83
1:A:735:ALA:HA	1:A:736:GLN:HB2	0.83	0.82
1:A:574:SER:HA	1:A:577:GLN:HG2	1.64	0.80
1:B:489:ILE:HG23	1:B:490:GLU:N	1.96	0.80
1:A:499:ARG:NH1	1:A:500:PHE:CE1	2.50	0.79
1:A:735:ALA:H	1:A:736:GLN:HG2	1.47	0.79
1:B:736:GLN:OE1	1:B:736:GLN:CA	2.30	0.78
1:B:734:GLU:CG	1:B:734:GLU:O	2.30	0.78
1:B:492:ILE:HG23	1:B:493:GLY:H	1.49	0.77
1:A:717:GLU:HG2	1:A:748:ARG:NH2	1.99	0.77
1:B:499:ARG:HH22	1:B:500:PHE:HZ	0.82	0.75
1:A:656:TRP:HH2	1:A:704:LEU:HD13	1.51	0.75
1:A:474:PHE:HB2	1:A:499:ARG:HD3	1.67	0.75
1:B:734:GLU:HG3	1:B:734:GLU:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ILE:CG2	1:B:490:GLU:H	2.00	0.74
1:A:736:GLN:HA	1:A:736:GLN:OE1	1.85	0.74
1:A:736:GLN:CA	1:A:736:GLN:OE1	2.36	0.74
1:B:574:SER:HA	1:B:577:GLN:HE21	1.53	0.74
1:A:451:PHE:CE1	1:A:535:ARG:CD	2.70	0.73
1:B:639:LYS:HB3	1:B:640:ASN:CG	2.10	0.72
1:B:474:PHE:HB2	1:B:499:ARG:HD3	1.72	0.71
1:A:734:GLU:HA	1:A:734:GLU:OE1	1.89	0.71
1:B:513:SER:HB3	1:B:602:VAL:HG22	1.72	0.71
1:A:664:VAL:HG21	1:A:690:HIS:HE1	1.56	0.70
1:B:557:MET:O	1:B:560:THR:HB	1.91	0.70
1:B:499:ARG:NH2	1:B:500:PHE:HZ	1.47	0.69
1:A:639:LYS:HB3	1:A:640:ASN:CG	2.14	0.68
1:B:681:GLN:O	1:B:682:ASP:OD1	2.12	0.68
1:B:492:ILE:HG23	1:B:493:GLY:N	2.08	0.68
1:B:638:PHE:HB3	1:B:641:LEU:HB2	1.76	0.68
1:A:735:ALA:N	1:A:736:GLN:CB	2.55	0.67
1:A:653:PRO:O	1:A:654:LEU:CD1	2.26	0.67
1:A:722:HIS:O	1:A:748:ARG:HD3	1.95	0.67
1:A:735:ALA:N	1:A:736:GLN:CG	2.58	0.67
1:A:664:VAL:HG21	1:A:690:HIS:CE1	2.30	0.66
1:A:632:ASP:OD2	1:A:705:ARG:HD3	1.97	0.63
1:B:492:ILE:CG2	1:B:493:GLY:H	2.10	0.63
1:A:735:ALA:H	1:A:736:GLN:CG	2.11	0.62
1:A:458:GLN:O	1:A:462:PRO:HA	2.00	0.62
1:B:617:ASP:HA	1:B:620:ARG:NH2	2.15	0.62
1:A:653:PRO:C	1:A:654:LEU:HD12	2.18	0.61
1:A:734:GLU:OE1	1:A:734:GLU:CA	2.48	0.61
1:A:423:GLU:O	1:A:427:THR:HG23	2.00	0.60
1:A:764:VAL:O	1:B:551:ARG:NH1	2.33	0.60
1:B:499:ARG:HH21	1:B:500:PHE:HE2	1.45	0.60
1:B:614:ARG:O	1:B:617:ASP:HB3	2.01	0.60
1:A:442:PHE:O	1:A:446:MET:HG3	2.02	0.60
1:A:668:VAL:HG22	1:A:677:LEU:HD23	1.84	0.60
1:B:460:ILE:C	1:B:462:PRO:HD3	2.23	0.59
1:B:626:HIS:HA	1:B:629:GLN:HG2	1.85	0.59
1:B:509:GLN:NE2	1:B:601:HIS:CG	2.71	0.58
1:B:689:SER:HG	1:B:689:SER:CB	2.08	0.58
1:B:445:PRO:HB2	1:B:539:PHE:HZ	1.70	0.57
1:B:623:ASP:HB3	1:B:686:LEU:HD13	1.86	0.57
1:A:551:ARG:NH1	1:A:551:ARG:HG3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HH11	1:A:551:ARG:HG3	1.69	0.56
1:B:735:ALA:HB1	1:B:736:GLN:O	2.05	0.56
1:B:574:SER:HA	1:B:577:GLN:NE2	2.19	0.56
1:A:646:LYS:HE2	1:A:674:LEU:HD12	1.86	0.56
1:A:714:MET:HE1	1:B:433:ARG:HB2	1.88	0.56
1:A:656:TRP:HH2	1:A:704:LEU:CD1	2.19	0.56
1:A:445:PRO:HB2	1:A:539:PHE:HZ	1.72	0.55
1:B:490:GLU:O	1:B:491:GLU:HB3	2.07	0.55
1:A:655:THR:HB	1:A:741:VAL:HG13	1.87	0.55
1:B:513:SER:CB	1:B:602:VAL:HG22	2.37	0.55
1:A:654:LEU:HD11	1:A:751:TRP:NE1	2.21	0.55
1:A:572:LEU:HB3	1:A:592:ALA:HB2	1.89	0.55
1:A:482:ARG:HD2	1:A:489:ILE:HD11	1.89	0.55
1:B:509:GLN:HE21	1:B:601:HIS:CG	2.23	0.55
1:A:453:PRO:HG2	1:A:456:GLU:HG3	1.89	0.55
1:A:710:LEU:C	1:A:712:SER:H	2.10	0.55
1:A:556:ASP:O	1:A:559:PRO:HD2	2.08	0.54
1:A:711:THR:HG22	1:A:762:LEU:HD23	1.90	0.54
1:A:656:TRP:CH2	1:A:704:LEU:HD13	2.39	0.54
1:A:513:SER:CB	1:A:602:VAL:HG22	2.38	0.53
1:A:736:GLN:OE1	1:A:736:GLN:N	2.42	0.53
1:A:717:GLU:HG2	1:A:748:ARG:HH21	1.71	0.53
1:B:492:ILE:CG2	1:B:493:GLY:N	2.71	0.53
1:A:748:ARG:HG3	1:A:749:LYS:N	2.24	0.52
1:A:656:TRP:HA	1:A:740:LEU:HD23	1.91	0.52
1:A:651:GLU:HA	1:A:668:VAL:O	2.10	0.52
1:B:734:GLU:O	1:B:735:ALA:C	2.48	0.52
1:A:735:ALA:H	1:A:736:GLN:HB2	1.71	0.52
1:B:468:ILE:O	1:B:472:SER:OG	2.21	0.52
1:B:474:PHE:CB	1:B:499:ARG:HD3	2.38	0.52
1:B:434:MET:HG3	1:B:435:LEU:N	2.24	0.51
1:A:691:SER:HB3	1:A:704:LEU:N	2.25	0.51
1:A:509:GLN:HE21	1:A:601:HIS:HB3	1.76	0.51
1:B:474:PHE:CG	1:B:499:ARG:HD3	2.46	0.51
1:B:617:ASP:HA	1:B:620:ARG:CZ	2.40	0.51
1:A:708:LEU:HB3	1:A:729:PHE:CE1	2.46	0.51
1:A:656:TRP:CH2	1:A:704:LEU:CD1	2.94	0.51
1:A:562:MET:HE1	1:A:606:VAL:HG21	1.93	0.51
1:B:459:ASN:O	1:B:518:ARG:HD3	2.11	0.51
1:B:724:ALA:HB2	1:B:741:VAL:HG22	1.93	0.50
1:B:722:HIS:O	1:B:745:VAL:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:O	1:A:712:SER:N	2.43	0.50
1:B:735:ALA:CB	1:B:736:GLN:HB2	2.31	0.50
1:B:462:PRO:HB2	1:B:515:PHE:HA	1.94	0.50
1:A:490:GLU:HG3	1:A:491:GLU:HG3	1.94	0.50
1:B:742:ALA:HB1	1:B:747:GLU:HG3	1.92	0.50
1:A:530:GLN:HE21	1:A:540:VAL:HG21	1.77	0.49
1:A:519:GLN:NE2	1:A:559:PRO:HB3	2.27	0.49
1:B:734:GLU:O	1:B:735:ALA:O	2.31	0.49
1:B:745:VAL:HG13	1:B:748:ARG:HH21	1.78	0.49
1:A:574:SER:HA	1:A:577:GLN:CG	2.40	0.49
1:A:639:LYS:HG2	1:A:640:ASN:HB3	1.95	0.49
1:A:490:GLU:HG3	1:A:491:GLU:N	2.28	0.49
1:B:683:GLU:HA	1:B:683:GLU:OE1	2.12	0.48
1:A:623:ASP:HA	1:A:684:ARG:HH21	1.78	0.48
1:A:639:LYS:HB3	1:A:640:ASN:CB	2.43	0.48
1:B:726:TYR:CE1	1:B:739:GLU:HG3	2.48	0.48
1:B:527:LYS:HD2	1:B:531:ARG:HH21	1.78	0.48
1:A:455:GLU:N	1:A:455:GLU:OE1	2.43	0.48
1:A:744:THR:HG22	1:A:747:GLU:OE1	2.13	0.47
1:B:458:GLN:O	1:B:462:PRO:HA	2.14	0.47
1:B:521:PHE:CE2	1:B:525:GLN:HG3	2.49	0.47
1:B:481:ARG:O	1:B:484:GLU:HG2	2.14	0.47
1:B:451:PHE:HE1	1:B:535:ARG:HG2	1.80	0.47
1:B:720:THR:O	1:B:721:ASP:HB2	2.15	0.47
1:A:491:GLU:HA	1:A:584:GLU:OE2	2.15	0.47
1:B:437:VAL:HG13	1:B:441:LEU:HD22	1.96	0.47
1:B:686:LEU:HD12	1:B:687:LEU:H	1.79	0.47
1:A:689:SER:HA	1:A:706:PRO:HD3	1.96	0.47
1:A:491:GLU:HA	1:A:584:GLU:CD	2.35	0.47
1:B:627:LEU:HD23	1:B:638:PHE:O	2.15	0.47
1:A:573:GLN:HE21	1:A:596:ARG:HD3	1.79	0.46
1:B:626:HIS:ND1	1:B:686:LEU:HD11	2.30	0.46
1:A:477:ARG:HB3	1:A:495:VAL:HG13	1.97	0.46
1:B:442:PHE:O	1:B:446:MET:HG3	2.15	0.46
1:A:647:LYS:HB2	1:A:672:ASP:HB3	1.98	0.46
1:B:735:ALA:HA	1:B:736:GLN:CG	2.34	0.46
1:A:438:LEU:HD13	1:A:557:MET:HB3	1.96	0.45
1:A:509:GLN:NE2	1:A:601:HIS:CG	2.84	0.45
1:A:638:PHE:HB3	1:A:641:LEU:HB2	1.98	0.45
1:A:529:LYS:HB3	1:A:536:PHE:CD2	2.51	0.45
1:A:499:ARG:HH21	1:A:500:PHE:HE2	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:GLN:C	1:B:682:ASP:CG	2.75	0.45
1:B:686:LEU:HD12	1:B:687:LEU:N	2.32	0.45
1:B:683:GLU:OE1	1:B:683:GLU:O	2.35	0.45
1:A:464:LEU:HA	1:A:464:LEU:HD12	1.61	0.45
1:A:744:THR:HG23	1:A:747:GLU:H	1.82	0.45
1:B:710:LEU:O	1:B:712:SER:N	2.49	0.45
1:B:649:VAL:HG12	1:B:650:HIS:HB2	1.98	0.45
1:B:684:ARG:O	1:B:685:LEU:HD23	2.17	0.45
1:B:558:ILE:N	1:B:559:PRO:HD2	2.31	0.44
1:A:444:GLN:HB3	1:A:445:PRO:HD3	1.98	0.44
1:A:497:LEU:HD12	1:A:591:ALA:HB2	2.00	0.44
1:B:632:ASP:OD2	1:B:705:ARG:NH1	2.50	0.44
1:A:553:GLN:OE1	1:A:555:LYS:HE2	2.18	0.44
1:A:735:ALA:H	1:A:736:GLN:CB	2.25	0.44
1:B:460:ILE:O	1:B:462:PRO:HD3	2.18	0.44
1:B:493:GLY:O	1:B:496:LEU:HB2	2.18	0.44
1:B:683:GLU:OE1	1:B:683:GLU:CA	2.65	0.44
1:A:724:ALA:HB2	1:A:741:VAL:HB	2.00	0.43
1:B:658:VAL:HG23	1:B:704:LEU:HD12	2.00	0.43
1:A:729:PHE:CD2	1:A:729:PHE:N	2.86	0.43
1:B:462:PRO:HG2	1:B:518:ARG:HB2	2.00	0.43
1:A:463:SER:O	1:A:464:LEU:C	2.56	0.43
1:B:509:GLN:NE2	1:B:601:HIS:HB3	2.33	0.43
1:A:533:ASP:HA	1:A:534:PRO:HD2	1.84	0.43
1:B:572:LEU:HB3	1:B:592:ALA:HB2	2.00	0.43
1:B:444:GLN:HB3	1:B:445:PRO:CD	2.41	0.43
1:B:714:MET:HB2	1:B:714:MET:HE2	1.69	0.43
1:B:500:PHE:CZ	1:B:595:CYS:SG	3.12	0.43
1:B:734:GLU:HG2	1:B:734:GLU:O	2.16	0.43
1:A:654:LEU:HD11	1:A:751:TRP:CE2	2.54	0.43
1:B:656:TRP:HB3	1:B:664:VAL:HB	2.01	0.42
1:B:551:ARG:NH1	1:B:551:ARG:HG3	2.35	0.42
1:A:659:THR:C	1:A:661:ASP:H	2.22	0.42
1:B:489:ILE:CG2	1:B:490:GLU:N	2.65	0.42
1:B:744:THR:HG22	1:B:747:GLU:CD	2.40	0.42
1:A:518:ARG:O	1:A:521:PHE:HB3	2.19	0.42
1:A:562:MET:O	1:A:563:GLN:C	2.58	0.42
1:A:726:TYR:CE1	1:A:739:GLU:HG3	2.55	0.42
1:A:517:SER:HA	1:A:606:VAL:HG22	2.02	0.41
1:B:509:GLN:NE2	1:B:601:HIS:CB	2.82	0.41
1:B:764:VAL:HG22	1:B:765:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LEU:HD13	1:A:685:LEU:HD13	2.00	0.41
1:A:635:LEU:HD21	1:A:705:ARG:HD2	2.02	0.41
1:A:521:PHE:CE2	1:A:525:GLN:HG3	2.55	0.41
1:B:764:VAL:CG2	1:B:765:PRO:HD2	2.50	0.41
1:B:639:LYS:HB3	1:B:640:ASN:CB	2.50	0.41
1:B:681:GLN:O	1:B:682:ASP:CG	2.58	0.41
1:A:747:GLU:O	1:A:750:ASN:HB3	2.21	0.41
1:B:646:LYS:HD3	1:B:671:LEU:HD23	2.03	0.41
1:B:674:LEU:HD11	1:B:709:ARG:NH1	2.35	0.41
1:B:721:ASP:C	1:B:723:LYS:H	2.24	0.41
1:A:639:LYS:HB3	1:A:640:ASN:HB3	2.03	0.41
1:A:511:ILE:HA	1:A:511:ILE:HD13	1.88	0.41
1:A:619:GLN:HG2	1:A:644:THR:HG23	2.03	0.41
1:A:635:LEU:CD2	1:A:705:ARG:HD2	2.51	0.41
1:A:513:SER:HB2	1:A:602:VAL:HG22	2.02	0.41
1:B:656:TRP:HA	1:B:740:LEU:HD23	2.03	0.40
1:A:566:THR:HG22	1:A:599:LEU:HD11	2.04	0.40
1:A:623:ASP:HA	1:A:684:ARG:NH2	2.35	0.40
1:B:616:LYS:HA	1:B:644:THR:HG22	2.02	0.40
1:B:708:LEU:HD21	1:B:738:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	326/417 (78%)	289 (89%)	30 (9%)	7 (2%)	8	42
1	B	327/417 (78%)	285 (87%)	32 (10%)	10 (3%)	5	31
All	All	653/834 (78%)	574 (88%)	62 (10%)	17 (3%)	6	36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	493	GLY
1	B	721	ASP
1	A	711	THR
1	A	736	GLN
1	B	490	GLU
1	B	492	ILE
1	B	560	THR
1	B	735	ALA
1	B	736	GLN
1	A	491	GLU
1	A	519	GLN
1	A	735	ALA
1	B	711	THR
1	A	761	SER
1	B	491	GLU
1	A	492	ILE
1	B	582	PRO

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	310/379 (82%)	295 (95%)	15 (5%)	30	68
1	B	309/379 (82%)	293 (95%)	16 (5%)	27	65
All	All	619/758 (82%)	588 (95%)	31 (5%)	28	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LYS
1	A	422	SER
1	A	450	LEU
1	A	463	SER
1	A	499	ARG
1	A	513	SER
1	A	535	ARG

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Mol	Chain	Res	Type
1	A	631	SER
1	A	640	ASN
1	A	656	TRP
1	A	682	ASP
1	A	689	SER
1	A	734	GLU
1	A	736	GLN
1	A	748	ARG
1	B	462	PRO
1	B	482	ARG
1	B	485	SER
1	B	499	ARG
1	B	529	LYS
1	B	535	ARG
1	B	627	LEU
1	B	640	ASN
1	B	661	ASP
1	B	665	GLU
1	B	682	ASP
1	B	683	GLU
1	B	688	LYS
1	B	714	MET
1	B	736	GLN
1	B	758	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	GLN
1	A	519	GLN
1	A	530	GLN
1	A	573	GLN
1	A	626	HIS
1	B	458	GLN
1	B	509	GLN
1	B	519	GLN
1	B	577	GLN

5.3.3 RNA ⓘ

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 [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	336/417 (80%)	-0.17	4 (1%)	79 67	67, 100, 155, 194	0
1	B	335/417 (80%)	-0.16	4 (1%)	79 67	72, 106, 193, 261	0
All	All	671/834 (80%)	-0.17	8 (1%)	79 67	67, 103, 173, 261	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	677	LEU	3.9
1	A	677	LEU	3.2
1	B	704	LEU	3.1
1	A	704	LEU	2.6
1	A	627	LEU	2.6
1	B	663	ALA	2.5
1	A	687	LEU	2.3
1	B	687	LEU	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.