



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2021 – 04:10 PM JST

PDB ID : 7CSR  
Title : Structure of Ephexin4 R676L  
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Deposited on : 2020-08-17  
Resolution : 3.00 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](mailto: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.

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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	:	2.16
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)	:	2.16

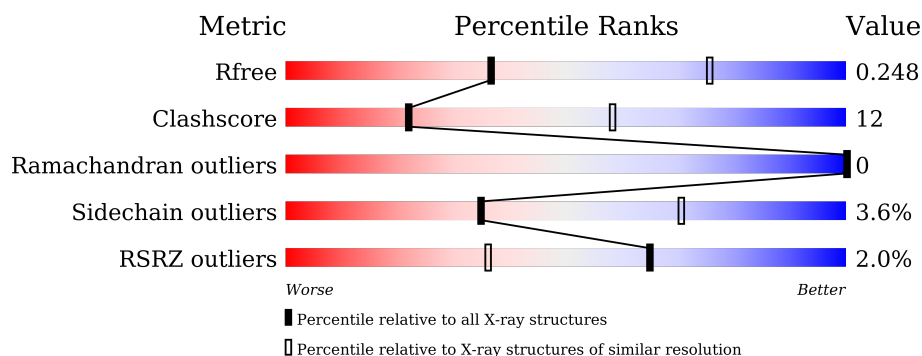
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	459	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 69%; height: 10px; background-color: green;"></div> <div style="width: 22%; height: 10px; background-color: yellow;"></div> <div style="width: 7%; height: 10px; background-color: orange;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>69%</span> <span>22%</span> <span>• 7%</span> </div> </div>
1	B	459	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>4%</span> <div style="width: 70%; height: 10px; background-color: green;"></div> <div style="width: 19%; height: 10px; background-color: yellow;"></div> <div style="width: 9%; height: 10px; background-color: orange;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>70%</span> <span>19%</span> <span>• 9%</span> </div> </div>
1	C	459	<div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 73%; height: 10px; background-color: green;"></div> <div style="width: 21%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>73%</span> <span>21%</span> <span>• 6%</span> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10175 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 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3406	2161	590	642	13			
1	B	418	Total	C	N	O	S	0	0	0
			3330	2114	568	636	12			
1	C	432	Total	C	N	O	S	0	0	0
			3439	2186	593	648	12			

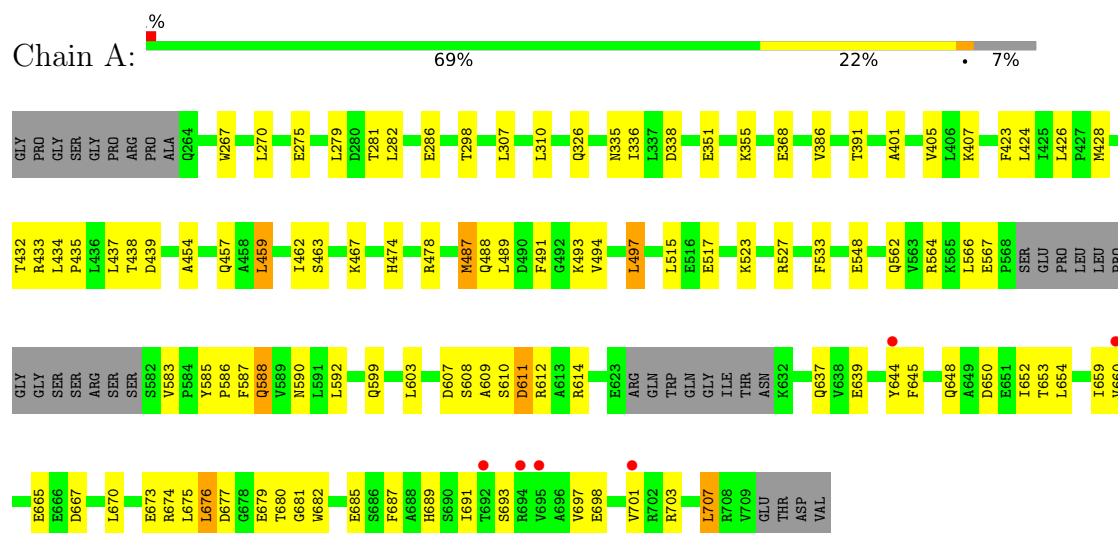
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLY	-	expression tag	UNP Q3U5C8
A	256	PRO	-	expression tag	UNP Q3U5C8
A	257	GLY	-	expression tag	UNP Q3U5C8
A	258	SER	-	expression tag	UNP Q3U5C8
A	259	GLY	-	expression tag	UNP Q3U5C8
A	260	PRO	-	expression tag	UNP Q3U5C8
A	676	LEU	ARG	engineered mutation	UNP Q3U5C8
B	255	GLY	-	expression tag	UNP Q3U5C8
B	256	PRO	-	expression tag	UNP Q3U5C8
B	257	GLY	-	expression tag	UNP Q3U5C8
B	258	SER	-	expression tag	UNP Q3U5C8
B	259	GLY	-	expression tag	UNP Q3U5C8
B	260	PRO	-	expression tag	UNP Q3U5C8
B	676	LEU	ARG	engineered mutation	UNP Q3U5C8
C	255	GLY	-	expression tag	UNP Q3U5C8
C	256	PRO	-	expression tag	UNP Q3U5C8
C	257	GLY	-	expression tag	UNP Q3U5C8
C	258	SER	-	expression tag	UNP Q3U5C8
C	259	GLY	-	expression tag	UNP Q3U5C8
C	260	PRO	-	expression tag	UNP Q3U5C8
C	676	LEU	ARG	engineered mutation	UNP Q3U5C8

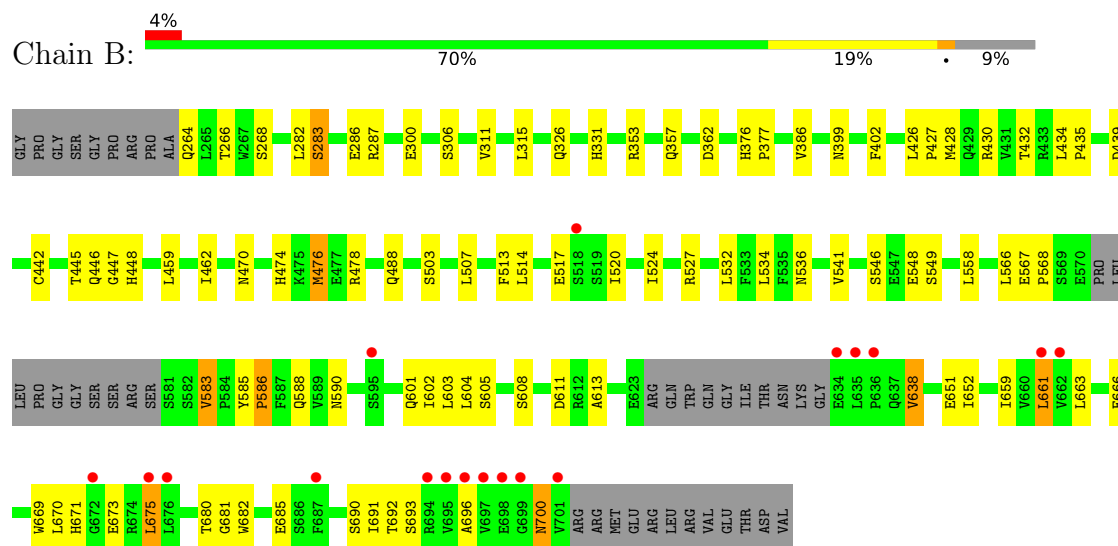
### 3 Residue-property plots

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 16

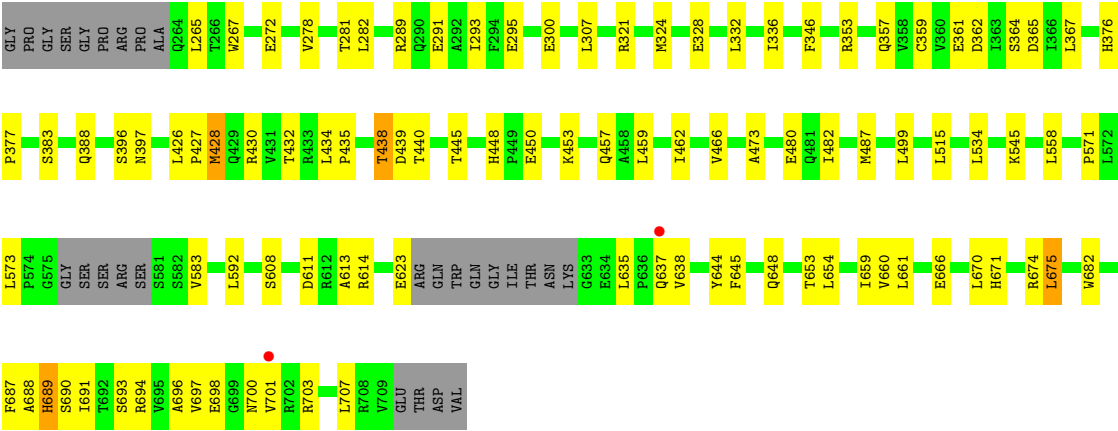


- Molecule 1: Rho guanine nucleotide exchange factor 16



- Molecule 1: Rho guanine nucleotide exchange factor 16





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.07Å 244.73Å 141.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.77 – 3.00 36.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.77-3.00) 99.3 (36.77-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.212 , 0.255 0.226 , 0.248	Depositor DCC
$R_{free}$ test set	2594 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.035 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10175	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.66	0/3472	0.76	1/4700 (0.0%)
1	B	0.74	5/3395 (0.1%)	0.76	1/4600 (0.0%)
1	C	0.62	0/3507	0.74	1/4750 (0.0%)
All	All	0.67	5/10374 (0.0%)	0.75	3/14050 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	PRO	N-CA	12.61	1.68	1.47
1	B	583	VAL	C-N	8.59	1.50	1.34
1	B	448	HIS	C-N	8.27	1.50	1.34
1	B	527	ARG	C-N	8.21	1.49	1.34
1	B	585	TYR	C-N	5.53	1.44	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	586	PRO	CA-N-CD	-7.36	101.20	111.50
1	A	650	ASP	CB-CA-C	-6.29	97.83	110.40
1	C	397	ASN	CB-CA-C	-5.02	100.35	110.40

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	3406	0	3366	80	1
1	B	3330	0	3270	77	2
1	C	3439	0	3401	83	1
All	All	10175	0	10037	239	2

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 12.

All (239) 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:586:PRO:N	1:B:586:PRO:CA	1.68	1.34
1:B:566:LEU:CD1	1:B:588:GLN:HB2	1.79	1.12
1:A:676:LEU:HD12	1:A:676:LEU:H	1.27	0.99
1:B:566:LEU:HD13	1:B:588:GLN:HB2	0.98	0.98
1:B:566:LEU:HD13	1:B:588:GLN:CB	1.94	0.93
1:B:661:LEU:HD21	1:B:675:LEU:CD1	1.98	0.93
1:A:608:SER:HB3	1:A:611:ASP:HB2	1.51	0.93
1:C:635:LEU:HD11	1:C:661:LEU:HB3	1.53	0.90
1:A:610:SER:HB3	1:A:667:ASP:HB3	1.55	0.88
1:C:278:VAL:CG1	1:C:282:LEU:HD13	2.03	0.87
1:B:474:HIS:O	1:B:478:ARG:HG3	1.74	0.87
1:B:661:LEU:HD21	1:B:675:LEU:HD12	1.55	0.86
1:C:661:LEU:HG	1:C:675:LEU:CD2	2.07	0.85
1:B:476:MET:HA	1:B:476:MET:HE3	1.57	0.84
1:B:428:MET:O	1:B:432:THR:HG23	1.79	0.82
1:B:661:LEU:CD2	1:B:675:LEU:HD12	2.10	0.81
1:A:707:LEU:HD12	1:A:707:LEU:H	1.46	0.80
1:B:520:ILE:H	1:B:520:ILE:HD12	1.47	0.79
1:A:645:PHE:HA	1:A:653:THR:HG23	1.63	0.78
1:A:652:ILE:HB	1:A:681:GLY:HA3	1.67	0.77
1:C:462:ILE:O	1:C:466:VAL:HG23	1.86	0.76
1:A:676:LEU:HD12	1:A:676:LEU:N	2.01	0.76
1:A:707:LEU:N	1:A:707:LEU:HD12	2.00	0.76
1:A:659:ILE:N	1:A:659:ILE:HD12	2.03	0.73
1:A:282:LEU:HD11	1:A:286:GLU:HG2	1.69	0.72
1:C:653:THR:O	1:C:674:ARG:NH1	2.23	0.72
1:B:520:ILE:N	1:B:520:ILE:HD12	2.04	0.72
1:A:676:LEU:H	1:A:676:LEU:CD1	2.01	0.71
1:A:428:MET:O	1:A:432:THR:HG23	1.89	0.71
1:C:435:PRO:HA	1:C:438:THR:HG22	1.71	0.71
1:A:698:GLU:HA	1:A:701:VAL:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:ILE:HD11	1:A:674:ARG:HB2	1.72	0.69
1:C:515:LEU:HD21	1:C:583:VAL:HG21	1.74	0.69
1:C:278:VAL:HG12	1:C:282:LEU:HD13	1.75	0.68
1:A:673:GLU:HB2	1:A:680:THR:HG22	1.75	0.68
1:C:654:LEU:HD23	1:C:674:ARG:HH11	1.57	0.68
1:A:567:GLU:HA	1:A:567:GLU:OE1	1.92	0.68
1:A:566:LEU:HB2	1:A:586:PRO:HB2	1.74	0.67
1:B:546:SER:HB3	1:B:549:SER:HB3	1.75	0.67
1:C:438:THR:HG21	1:C:462:ILE:HG21	1.75	0.67
1:B:586:PRO:C	1:B:586:PRO:N	2.46	0.66
1:A:489:LEU:HD11	1:A:533:PHE:CE1	2.29	0.66
1:C:661:LEU:HG	1:C:675:LEU:HD21	1.75	0.66
1:C:300:GLU:OE1	1:C:430:ARG:NH2	2.26	0.66
1:C:346:PHE:HZ	1:C:367:LEU:HD23	1.61	0.65
1:C:281:THR:O	1:C:281:THR:OG1	2.11	0.65
1:B:524:ILE:C	1:B:524:ILE:HD12	2.17	0.65
1:B:670:LEU:HD11	1:B:685:GLU:HB3	1.79	0.64
1:B:546:SER:HB3	1:B:549:SER:CB	2.26	0.64
1:C:698:GLU:HA	1:C:701:VAL:HG12	1.79	0.64
1:C:364:SER:HA	1:C:367:LEU:HD12	1.80	0.64
1:C:459:LEU:HD11	1:C:707:LEU:HD22	1.78	0.64
1:B:524:ILE:O	1:B:524:ILE:HD12	1.98	0.64
1:A:659:ILE:HB	1:A:675:LEU:HD13	1.80	0.63
1:B:434:LEU:N	1:B:435:PRO:HD2	2.13	0.63
1:C:289:ARG:O	1:C:293:ILE:HG13	2.00	0.62
1:A:435:PRO:HA	1:A:438:THR:HG22	1.82	0.62
1:C:434:LEU:N	1:C:435:PRO:HD2	2.15	0.62
1:A:585:TYR:N	1:A:586:PRO:HD3	2.15	0.61
1:B:476:MET:CE	1:B:476:MET:HA	2.27	0.61
1:C:289:ARG:NH1	1:C:289:ARG:HG2	2.16	0.61
1:B:673:GLU:HB2	1:B:680:THR:HG22	1.83	0.61
1:A:281:THR:O	1:A:281:THR:HG23	2.01	0.61
1:B:282:LEU:HD23	1:B:287:ARG:HB2	1.83	0.60
1:B:700:ASN:N	1:B:700:ASN:HD22	1.99	0.60
1:C:445:THR:O	1:C:445:THR:HG22	2.01	0.60
1:C:691:ILE:HG22	1:C:697:VAL:CG1	2.31	0.60
1:A:434:LEU:N	1:A:435:PRO:HD2	2.16	0.59
1:C:661:LEU:HG	1:C:675:LEU:HD22	1.81	0.59
1:C:376:HIS:N	1:C:377:PRO:HD2	2.16	0.59
1:A:583:VAL:O	1:A:583:VAL:HG23	2.01	0.59
1:A:677:ASP:OD1	1:A:677:ASP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ARG:O	1:A:707:LEU:CD1	2.51	0.58
1:B:445:THR:HG22	1:B:445:THR:O	2.04	0.58
1:B:520:ILE:CD1	1:B:520:ILE:H	2.16	0.58
1:B:661:LEU:CG	1:B:675:LEU:HD12	2.34	0.58
1:B:583:VAL:HG23	1:B:583:VAL:O	2.03	0.58
1:A:515:LEU:HD11	1:A:583:VAL:HG21	1.87	0.57
1:B:566:LEU:CD1	1:B:588:GLN:CB	2.71	0.57
1:A:648:GLN:OE1	1:A:648:GLN:HA	2.03	0.57
1:C:545:LYS:HE2	1:C:545:LYS:HA	1.87	0.57
1:A:368:GLU:OE2	1:A:457:GLN:HB3	2.05	0.56
1:A:564:ARG:HG3	1:C:592:LEU:HD22	1.88	0.56
1:C:353:ARG:NH2	1:C:365:ASP:OD2	2.21	0.56
1:A:433:ARG:HE	1:A:437:LEU:HD21	1.69	0.56
1:A:335:ASN:HB2	1:A:338:ASP:HB2	1.88	0.56
1:A:587:PHE:CD1	1:A:612:ARG:HG3	2.40	0.55
1:B:306:SER:HB3	1:B:426:LEU:CD1	2.37	0.55
1:C:459:LEU:HD11	1:C:707:LEU:CD2	2.37	0.55
1:B:692:THR:OG1	1:B:692:THR:O	2.23	0.55
1:C:434:LEU:HD13	1:C:462:ILE:HD11	1.88	0.55
1:B:613:ALA:HB2	1:B:666:GLU:HG2	1.88	0.54
1:A:588:GLN:HG3	1:A:603:LEU:HG	1.88	0.54
1:A:703:ARG:O	1:A:707:LEU:HD12	2.08	0.54
1:C:638:VAL:HG12	1:C:660:VAL:O	2.07	0.54
1:B:602:ILE:HG22	1:B:604:LEU:HG	1.87	0.54
1:B:638:VAL:HG23	1:B:690:SER:HA	1.90	0.54
1:C:289:ARG:CG	1:C:289:ARG:HH11	2.21	0.54
1:A:675:LEU:C	1:A:675:LEU:HD23	2.29	0.54
1:C:700:ASN:OD1	1:C:703:ARG:NH2	2.29	0.53
1:C:614:ARG:HG2	1:C:682:TRP:CE2	2.43	0.53
1:C:383:SER:HA	1:C:473:ALA:HA	1.89	0.53
1:A:474:HIS:O	1:A:478:ARG:HG2	2.09	0.53
1:B:652:ILE:HG23	1:B:652:ILE:O	2.08	0.52
1:C:638:VAL:HG22	1:C:688:ALA:HB1	1.91	0.52
1:C:324:MET:HB2	1:C:328:GLU:HB2	1.91	0.52
1:B:476:MET:CE	1:B:476:MET:CA	2.85	0.52
1:B:588:GLN:HG3	1:B:603:LEU:HD23	1.92	0.52
1:A:652:ILE:HG23	1:A:652:ILE:O	2.09	0.52
1:B:399:ASN:HB3	1:B:402:PHE:HB3	1.92	0.52
1:C:571:PRO:HB2	1:C:573:LEU:O	2.09	0.52
1:C:659:ILE:HG13	1:C:675:LEU:HB2	1.91	0.51
1:A:488:GLN:NE2	1:A:548:GLU:HG2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:GLN:NE2	1:C:359:CYS:O	2.43	0.51
1:C:353:ARG:NH1	1:C:362:ASP:O	2.42	0.51
1:B:300:GLU:OE1	1:B:430:ARG:NH2	2.28	0.51
1:B:459:LEU:HA	1:B:462:ILE:HG22	1.93	0.51
1:A:351:GLU:HG2	1:A:355:LYS:HD3	1.92	0.51
1:C:448:HIS:NE2	1:C:450:GLU:HB3	2.26	0.51
1:C:534:LEU:HD11	1:C:558:LEU:HD13	1.93	0.50
1:B:651:GLU:HA	1:B:682:TRP:H	1.77	0.50
1:A:644:TYR:HB2	1:A:687:PHE:CD2	2.47	0.50
1:C:608:SER:HB3	1:C:611:ASP:H	1.77	0.50
1:C:693:SER:HB3	1:C:696:ALA:HB3	1.94	0.50
1:B:693:SER:HB2	1:B:696:ALA:CB	2.42	0.50
1:B:700:ASN:N	1:B:700:ASN:ND2	2.60	0.49
1:C:691:ILE:HG22	1:C:697:VAL:HG13	1.94	0.49
1:B:661:LEU:HG	1:B:675:LEU:HD12	1.95	0.49
1:C:289:ARG:CG	1:C:289:ARG:NH1	2.73	0.49
1:A:487:MET:O	1:A:487:MET:HG2	2.10	0.49
1:A:267:TRP:HA	1:A:270:LEU:HG	1.94	0.48
1:A:562:GLN:HB2	1:A:590:ASN:HB2	1.94	0.48
1:C:648:GLN:HA	1:C:648:GLN:OE1	2.13	0.48
1:C:635:LEU:CD1	1:C:661:LEU:HB3	2.36	0.48
1:A:687:PHE:N	1:A:687:PHE:CD1	2.80	0.48
1:B:659:ILE:HG13	1:B:659:ILE:O	2.12	0.48
1:B:691:ILE:HG23	1:B:691:ILE:O	2.13	0.48
1:C:623:GLU:N	1:C:623:GLU:OE1	2.46	0.48
1:C:638:VAL:CG1	1:C:660:VAL:HB	2.44	0.48
1:A:438:THR:HG23	1:A:459:LEU:HD13	1.94	0.48
1:A:401:ALA:O	1:A:405:VAL:HG23	2.14	0.48
1:A:614:ARG:HG2	1:A:682:TRP:CE2	2.48	0.48
1:C:645:PHE:HA	1:C:653:THR:HG23	1.94	0.48
1:C:661:LEU:CG	1:C:675:LEU:HD21	2.43	0.48
1:B:671:HIS:HB2	1:B:682:TRP:CZ2	2.49	0.48
1:B:566:LEU:HB3	1:B:586:PRO:HB2	1.95	0.47
1:A:326:GLN:CD	1:A:326:GLN:H	2.18	0.47
1:B:353:ARG:NH1	1:B:362:ASP:O	2.48	0.47
1:A:433:ARG:O	1:A:433:ARG:HG2	2.14	0.47
1:A:585:TYR:CE1	1:A:609:ALA:HB2	2.50	0.47
1:B:671:HIS:HB2	1:B:682:TRP:CH2	2.49	0.47
1:B:652:ILE:HB	1:B:681:GLY:HA3	1.97	0.47
1:C:661:LEU:CD2	1:C:675:LEU:HD21	2.46	0.46
1:A:310:LEU:HD23	1:A:336:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:HIS:C	1:C:448:HIS:CD2	2.86	0.46
1:B:286:GLU:HA	1:B:286:GLU:OE1	2.16	0.46
1:B:514:LEU:HA	1:B:514:LEU:HD23	1.74	0.46
1:A:687:PHE:HD1	1:A:687:PHE:N	2.14	0.46
1:C:482:ILE:HA	1:C:482:ILE:HD12	1.82	0.46
1:B:520:ILE:CD1	1:B:520:ILE:N	2.74	0.46
1:C:434:LEU:HB3	1:C:462:ILE:HG12	1.98	0.45
1:C:637:GLN:HG2	1:C:661:LEU:HD23	1.98	0.45
1:C:438:THR:HG21	1:C:462:ILE:CG2	2.46	0.45
1:C:448:HIS:O	1:C:448:HIS:CD2	2.70	0.45
1:A:335:ASN:OD1	1:A:335:ASN:N	2.49	0.45
1:A:592:LEU:O	1:A:599:GLN:HG2	2.17	0.45
1:B:488:GLN:HG2	1:B:548:GLU:O	2.16	0.45
1:B:590:ASN:ND2	1:B:601:GLN:HG2	2.31	0.44
1:C:453:LYS:O	1:C:457:GLN:HG2	2.16	0.44
1:B:446:GLN:HG2	1:B:447:GLY:N	2.33	0.44
1:B:663:LEU:HB2	1:B:671:HIS:O	2.18	0.44
1:C:289:ARG:HH11	1:C:289:ARG:HG2	1.82	0.44
1:B:693:SER:HB2	1:B:696:ALA:HB2	2.00	0.44
1:C:691:ILE:HG22	1:C:697:VAL:HG12	2.00	0.44
1:C:295:GLU:O	1:C:295:GLU:HG3	2.17	0.44
1:B:590:ASN:HD22	1:B:601:GLN:HG2	1.83	0.44
1:C:426:LEU:HB2	1:C:427:PRO:HD3	1.98	0.44
1:C:694:ARG:NH1	1:C:694:ARG:HB3	2.33	0.43
1:A:566:LEU:HA	1:A:566:LEU:HD23	1.71	0.43
1:C:439:ASP:HB2	1:C:707:LEU:HD21	1.99	0.43
1:B:283:SER:HB2	1:B:286:GLU:H	1.84	0.43
1:C:426:LEU:N	1:C:427:PRO:CD	2.81	0.43
1:B:513:PHE:HB2	1:B:605:SER:O	2.18	0.43
1:B:661:LEU:HD23	1:B:661:LEU:N	2.32	0.43
1:C:689:HIS:ND1	1:C:689:HIS:C	2.72	0.43
1:A:659:ILE:H	1:A:659:ILE:HD12	1.81	0.43
1:C:638:VAL:HG12	1:C:660:VAL:HB	2.01	0.43
1:C:670:LEU:O	1:C:682:TRP:HA	2.18	0.43
1:A:491:PHE:CZ	1:A:497:LEU:HD23	2.53	0.43
1:B:376:HIS:N	1:B:377:PRO:CD	2.81	0.43
1:A:282:LEU:HD11	1:A:286:GLU:CG	2.43	0.43
1:B:264:GLN:N	1:B:264:GLN:CD	2.73	0.43
1:A:689:HIS:C	1:A:689:HIS:ND1	2.72	0.42
1:B:536:ASN:OD1	1:B:536:ASN:N	2.52	0.42
1:B:439:ASP:O	1:B:442:CYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:HIS:N	1:B:377:PRO:HD2	2.34	0.42
1:B:507:LEU:HD11	1:B:536:ASN:HA	2.01	0.42
1:B:602:ILE:CG2	1:B:604:LEU:HD21	2.50	0.42
1:A:691:ILE:HG22	1:A:697:VAL:HG22	2.02	0.42
1:A:654:LEU:HD11	1:A:660:VAL:HG21	2.01	0.42
1:A:637:GLN:NE2	1:A:701:VAL:HG13	2.35	0.42
1:B:532:LEU:CD2	1:B:541:VAL:HG13	2.50	0.42
1:C:693:SER:HB3	1:C:696:ALA:CB	2.50	0.42
1:C:267:TRP:N	1:C:291:GLU:OE2	2.51	0.42
1:C:307:LEU:HD22	1:C:336:ILE:HD11	2.01	0.42
1:C:499:LEU:HD12	1:C:499:LEU:HA	1.87	0.42
1:A:693:SER:O	1:A:697:VAL:HG23	2.20	0.42
1:A:310:LEU:HD21	1:A:424:LEU:HD23	2.01	0.41
1:C:332:LEU:O	1:C:388:GLN:NE2	2.47	0.41
1:A:467:LYS:HB3	1:A:467:LYS:HE3	1.88	0.41
1:C:289:ARG:NH2	1:C:361:GLU:O	2.53	0.41
1:C:434:LEU:N	1:C:435:PRO:CD	2.83	0.41
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.89	0.41
1:A:493:LYS:HG2	1:A:494:VAL:HG13	2.02	0.41
1:C:321:ARG:HD2	1:C:321:ARG:O	2.20	0.41
1:A:454:ALA:O	1:A:457:GLN:HB2	2.20	0.41
1:C:671:HIS:HB2	1:C:682:TRP:CE2	2.56	0.41
1:C:428:MET:O	1:C:432:THR:HG23	2.21	0.41
1:A:434:LEU:HB3	1:A:462:ILE:HD12	2.03	0.41
1:A:527:ARG:NH2	1:A:607:ASP:OD1	2.54	0.41
1:A:673:GLU:HA	1:A:680:THR:HA	2.02	0.41
1:B:567:GLU:HA	1:B:568:PRO:HD3	1.90	0.41
1:A:434:LEU:N	1:A:435:PRO:CD	2.82	0.41
1:B:426:LEU:N	1:B:427:PRO:CD	2.83	0.41
1:C:644:TYR:HB2	1:C:687:PHE:HD2	1.86	0.41
1:B:287:ARG:NH2	1:B:287:ARG:HG2	2.36	0.40
1:C:265:LEU:HA	1:C:265:LEU:HD12	1.97	0.40
1:A:307:LEU:HD22	1:A:336:ILE:HD11	2.03	0.40
1:A:459:LEU:O	1:A:459:LEU:HD12	2.21	0.40
1:A:639:GLU:HB2	1:A:691:ILE:HD11	2.02	0.40
1:B:311:VAL:HA	1:B:315:LEU:HB3	2.03	0.40
1:B:608:SER:HB3	1:B:611:ASP:HB2	2.03	0.40
1:A:439:ASP:HA	1:A:459:LEU:HD22	2.03	0.40
1:C:613:ALA:HB2	1:C:666:GLU:HG2	2.03	0.40
1:A:652:ILE:CG2	1:A:652:ILE:O	2.70	0.40
1:B:534:LEU:HD11	1:B:558:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:HA	1:A:426:LEU:HD12	2.03	0.40
1:A:434:LEU:HA	1:A:434:LEU:HD23	1.88	0.40
1:A:670:LEU:HG	1:A:685:GLU:HB3	2.03	0.40

All (2) 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:326:GLN:OE1	1:C:480:GLU:OE2[6_554]	2.07	0.13
1:A:523:LYS:NZ	1:B:357:GLN:O[8_457]	2.12	0.08

## 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	419/459 (91%)	407 (97%)	12 (3%)	0	100	100
1	B	412/459 (90%)	400 (97%)	12 (3%)	0	100	100
1	C	426/459 (93%)	413 (97%)	13 (3%)	0	100	100
All	All	1257/1377 (91%)	1220 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	374/411 (91%)	357 (96%)	17 (4%)	27	64
1	B	366/411 (89%)	352 (96%)	14 (4%)	33	69
1	C	377/411 (92%)	368 (98%)	9 (2%)	49	79
All	All	1117/1233 (91%)	1077 (96%)	40 (4%)	35	70

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLU
1	A	279	LEU
1	A	298	THR
1	A	386	VAL
1	A	391	THR
1	A	407	LYS
1	A	459	LEU
1	A	463	SER
1	A	487	MET
1	A	497	LEU
1	A	517	GLU
1	A	588	GLN
1	A	611	ASP
1	A	665	GLU
1	A	676	LEU
1	A	679	GLU
1	A	707	LEU
1	B	266	THR
1	B	268	SER
1	B	283	SER
1	B	331	HIS
1	B	386	VAL
1	B	470	ASN
1	B	476	MET
1	B	503	SER
1	B	517	GLU
1	B	638	VAL
1	B	661	LEU
1	B	669	TRP
1	B	675	LEU
1	B	700	ASN
1	C	272	GLU
1	C	396	SER
1	C	428	MET

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Mol	Chain	Res	Type
1	C	438	THR
1	C	440	THR
1	C	487	MET
1	C	675	LEU
1	C	689	HIS
1	C	690	SER

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

Mol	Chain	Res	Type
1	A	486	ASN
1	A	488	GLN
1	A	664	GLN
1	B	562	GLN
1	B	590	ASN
1	B	599	GLN
1	B	700	ASN
1	C	384	ASN
1	C	448	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 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/459 (92%)	-0.26	6 (1%) 75 49	30, 66, 112, 140	0
1	B	418/459 (91%)	-0.12	18 (4%) 35 13	31, 70, 119, 173	0
1	C	432/459 (94%)	-0.23	2 (0%) 91 75	34, 61, 121, 137	0
All	All	1275/1377 (92%)	-0.20	26 (2%) 65 36	30, 65, 118, 173	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	661	LEU	4.4
1	B	675	LEU	3.6
1	C	637	GLN	3.2
1	B	695	VAL	3.0
1	A	692	THR	3.0
1	B	595	SER	3.0
1	A	695	VAL	2.9
1	A	701	VAL	2.8
1	B	699	GLY	2.7
1	B	662	VAL	2.7
1	B	696	ALA	2.7
1	B	701	VAL	2.5
1	A	694	ARG	2.5
1	B	694	ARG	2.4
1	B	634	GLU	2.4
1	B	698	GLU	2.4
1	B	636	PRO	2.3
1	B	672	GLY	2.3
1	A	644	TYR	2.2
1	B	676	LEU	2.2
1	B	518	SER	2.2
1	B	635	LEU	2.2
1	C	701	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	687	PHE	2.1
1	B	697	VAL	2.1
1	A	660	VAL	2.1

## 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.