



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2RAI  
Title : The PX-BAR membrane remodeling unit of Sorting Nexin 9  
Authors : Pylypenko, O.; Lundmark, R.; Rasmuson, E.; Carlsson, S.R.; Rak, A.  
Deposited on : 2007-09-16  
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](mailto: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.

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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  
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

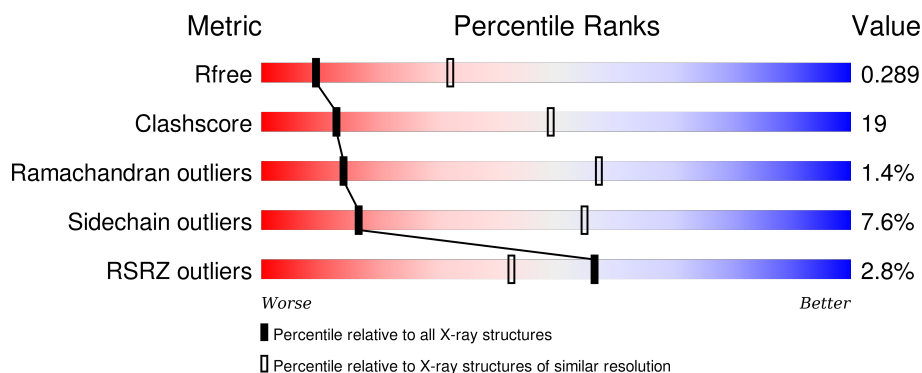
# 1 Overall quality at a glance

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  $\geq 3$ , 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	392	 2% 54% 35% • 7%
1	B	392	 3% 53% 37% • 6%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5919 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.

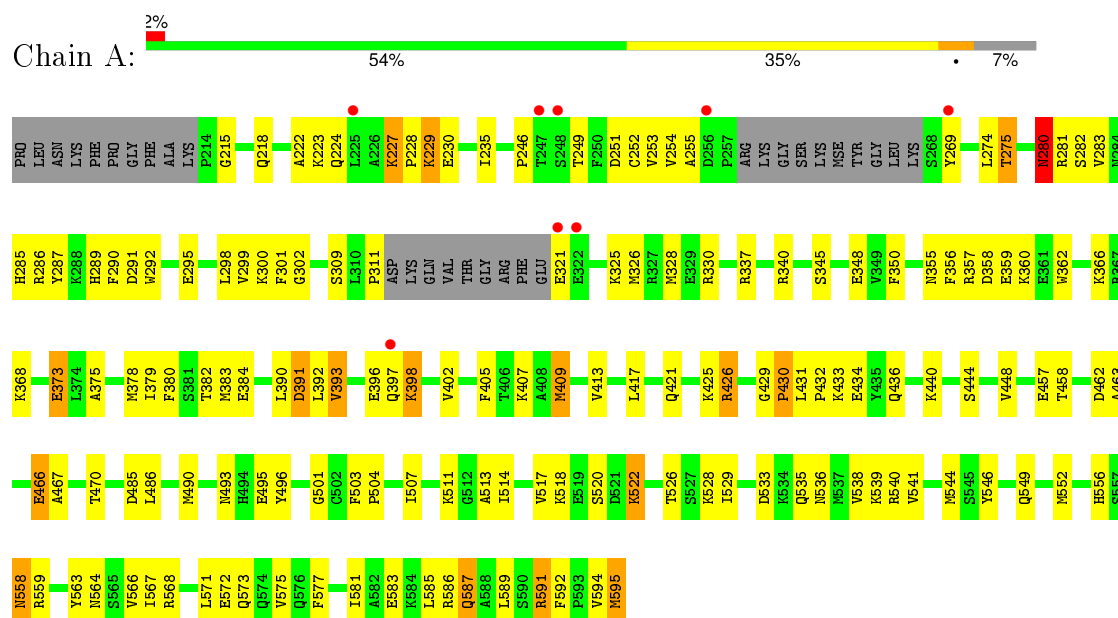
- Molecule 1 is a protein called Sorting nexin-9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	Se	0	0	0
			2947	1883	494	551	6	13			
1	B	368	Total	C	N	O	S	Se	0	0	0
			2972	1895	500	558	6	13			

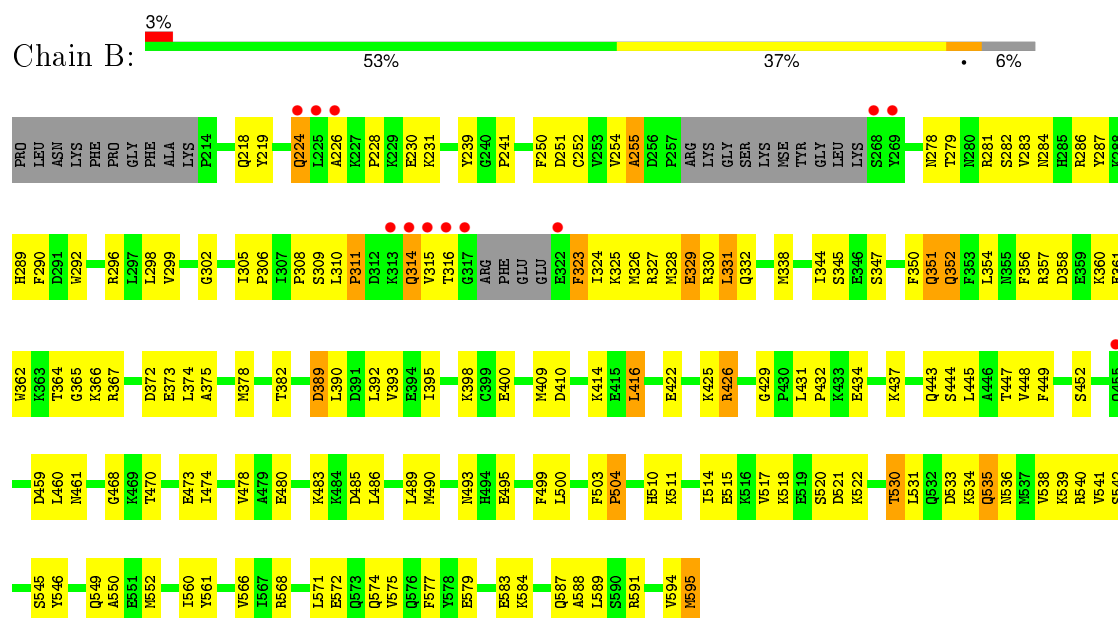
### 3 Residue-property plots

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: Sorting nexin-9



#### • Molecule 1: Sorting nexin-9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.63Å 117.55Å 145.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 3.20 19.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.76-3.20) 99.7 (19.76-3.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.18 (at 3.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.301 0.223 , 0.289	Depositor DCC
$R_{free}$ test set	955 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.6	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19093 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4935e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 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	0.52	0/3000	0.61	0/4022
1	B	0.49	0/3024	0.60	0/4056
All	All	0.51	0/6024	0.60	0/8078

There are no bond length outliers.

There are no bond angle outliers.

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	2947	0	2930	113	0
1	B	2972	0	2950	128	0
All	All	5919	0	5880	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 19.

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:531:LEU:HG	1:B:535:GLN:HE22	1.31	0.92
1:A:228:PRO:HG3	1:A:382:THR:HA	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:HE3	1:A:526:THR:HG21	1.62	0.80
1:B:409:MSE:HE2	1:B:500:LEU:HD11	1.63	0.80
1:B:426:ARG:NH1	1:B:426:ARG:HB2	1.99	0.77
1:A:345:SER:HA	1:A:350:PHE:CD2	2.22	0.73
1:A:595:MSE:HG3	1:B:561:TYR:HE1	1.54	0.73
1:A:280:ASN:ND2	1:A:280:ASN:H	1.86	0.72
1:A:227:LYS:H	1:A:227:LYS:HE2	1.56	0.71
1:A:431:LEU:HB3	1:A:432:PRO:HD3	1.73	0.70
1:B:315:VAL:HG12	1:B:316:THR:H	1.57	0.70
1:A:227:LYS:N	1:A:227:LYS:HE2	2.07	0.69
1:B:444:SER:O	1:B:448:VAL:HG23	1.91	0.69
1:B:392:LEU:HD11	1:B:517:VAL:HG12	1.74	0.69
1:B:255:ALA:HA	1:B:328:MSE:SE	2.42	0.68
1:A:255:ALA:HA	1:A:328:MSE:SE	2.43	0.68
1:B:324:ILE:HA	1:B:327:ARG:HB3	1.76	0.67
1:B:366:LYS:HG2	1:B:366:LYS:O	1.94	0.67
1:B:531:LEU:HG	1:B:535:GLN:NE2	2.08	0.66
1:B:351:GLN:HA	1:B:351:GLN:HE21	1.61	0.66
1:A:280:ASN:HD22	1:A:280:ASN:N	1.93	0.66
1:A:326:MSE:HE3	1:A:330:ARG:HH11	1.62	0.65
1:B:375:ALA:O	1:B:378:MSE:HB2	1.97	0.65
1:A:356:PHE:CD1	1:A:362:TRP:HB2	2.32	0.64
1:A:275:THR:HG23	1:A:282:SER:HB3	1.79	0.63
1:A:391:ASP:HB2	1:A:393:VAL:HG23	1.80	0.63
1:B:395:ILE:HD11	1:B:542:SER:HA	1.81	0.62
1:A:568:ARG:O	1:A:572:GLU:HG3	1.99	0.62
1:A:586:ARG:NH2	1:B:579:GLU:OE1	2.32	0.62
1:B:356:PHE:CD1	1:B:362:TRP:HB2	2.35	0.62
1:B:400:GLU:HG2	1:B:511:LYS:NZ	2.16	0.61
1:A:280:ASN:ND2	1:A:280:ASN:N	2.48	0.61
1:B:429:GLY:O	1:B:432:PRO:HD2	2.01	0.60
1:A:426:ARG:HB2	1:A:426:ARG:NH1	2.15	0.60
1:A:426:ARG:HD2	1:B:434:GLU:OE2	2.01	0.60
1:B:594:VAL:O	1:B:595:MSE:HB2	2.01	0.60
1:B:352:GLN:HE21	1:B:352:GLN:N	1.99	0.60
1:B:431:LEU:HB3	1:B:432:PRO:HD3	1.83	0.60
1:B:510:HIS:O	1:B:514:ILE:HG13	2.02	0.59
1:B:474:ILE:O	1:B:478:VAL:HG23	2.02	0.59
1:B:219:TYR:CE2	1:B:540:ARG:HB3	2.37	0.59
1:B:426:ARG:CZ	1:B:426:ARG:HB2	2.31	0.59
1:B:372:ASP:OD1	1:B:374:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:SER:HB2	1:B:534:LYS:HG3	1.84	0.59
1:B:347:SER:O	1:B:351:GLN:HG2	2.02	0.58
1:A:564:ASN:HD22	1:B:460:LEU:HD13	1.68	0.58
1:A:254:VAL:HG22	1:A:274:LEU:HD23	1.85	0.58
1:B:345:SER:HA	1:B:350:PHE:CD2	2.38	0.58
1:A:321:GLU:O	1:A:325:LYS:HG2	2.05	0.57
1:A:594:VAL:O	1:A:595:MSE:HB2	2.04	0.56
1:A:571:LEU:O	1:A:575:VAL:HG23	2.05	0.56
1:A:286:ARG:O	1:A:289:HIS:N	2.36	0.56
1:B:530:THR:HG23	1:B:533:ASP:OD1	2.05	0.56
1:B:422:GLU:HA	1:B:425:LYS:HE3	1.87	0.56
1:A:444:SER:O	1:A:448:VAL:HG23	2.05	0.56
1:A:457:GLU:HG3	1:B:560:ILE:HD11	1.87	0.56
1:A:556:HIS:ND1	1:A:559:ARG:NH2	2.51	0.55
1:B:224:GLN:HA	1:B:224:GLN:OE1	2.05	0.55
1:B:489:LEU:HA	1:B:566:VAL:HG21	1.88	0.55
1:B:360:LYS:O	1:B:364:THR:HG22	2.07	0.55
1:B:514:ILE:HG22	1:B:518:LYS:HE3	1.88	0.54
1:A:496:TYR:OH	1:A:559:ARG:HA	2.06	0.54
1:A:215:GLY:O	1:A:218:GLN:HB3	2.06	0.54
1:B:281:ARG:CZ	1:B:357:ARG:HH21	2.19	0.54
1:A:434:GLU:OE1	1:B:426:ARG:HD2	2.07	0.54
1:A:380:PHE:CE2	1:A:544:MSE:HE3	2.43	0.54
1:A:396:GLU:HG3	1:A:514:ILE:HG21	1.90	0.54
1:B:298:LEU:O	1:B:302:GLY:HA3	2.08	0.53
1:B:389:ASP:OD2	1:B:539:LYS:HG2	2.07	0.53
1:A:398:LYS:NZ	1:A:398:LYS:HB2	2.23	0.53
1:B:485:ASP:OD2	1:B:486:LEU:N	2.37	0.53
1:A:536:ASN:O	1:A:540:ARG:HG3	2.08	0.53
1:B:314:GLN:NE2	1:B:323:PHE:HA	2.24	0.53
1:B:514:ILE:O	1:B:518:LYS:HG3	2.09	0.52
1:B:390:LEU:HG	1:B:546:TYR:CE1	2.44	0.52
1:B:410:ASP:O	1:B:414:LYS:HB2	2.09	0.52
1:A:592:PHE:O	1:B:568:ARG:NH1	2.42	0.52
1:A:493:ASN:ND2	1:A:563:TYR:OH	2.42	0.52
1:A:254:VAL:HG22	1:A:274:LEU:CD2	2.39	0.52
1:A:375:ALA:O	1:A:378:MSE:HB2	2.10	0.52
1:B:251:ASP:CG	1:B:252:CYS:H	2.13	0.51
1:B:279:THR:O	1:B:281:ARG:HG3	2.10	0.51
1:A:373:GLU:H	1:A:373:GLU:CD	2.13	0.51
1:A:409:MSE:O	1:A:413:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:GLU:HA	1:B:329:GLU:OE1	2.10	0.51
1:B:521:ASP:OD1	1:B:534:LYS:HE3	2.11	0.51
1:A:227:LYS:H	1:A:227:LYS:CE	2.24	0.51
1:A:535:GLN:HB3	1:A:539:LYS:HE3	1.91	0.51
1:A:311:PRO:HG3	1:A:330:ARG:CB	2.40	0.51
1:B:241:PRO:HG2	1:B:549:GLN:CB	2.41	0.51
1:A:485:ASP:HB3	1:A:573:GLN:HB2	1.93	0.51
1:B:426:ARG:HH11	1:B:426:ARG:HB2	1.76	0.50
1:A:589:LEU:HD21	1:B:572:GLU:HG2	1.93	0.50
1:B:352:GLN:HE21	1:B:352:GLN:H	1.60	0.50
1:B:241:PRO:HG2	1:B:549:GLN:HB2	1.94	0.49
1:A:246:PRO:HG2	1:A:249:THR:HG22	1.93	0.49
1:A:485:ASP:OD2	1:A:486:LEU:N	2.40	0.49
1:B:292:TRP:O	1:B:296:ARG:HG2	2.12	0.49
1:B:331:LEU:HD23	1:B:331:LEU:O	2.11	0.49
1:B:311:PRO:HG3	1:B:330:ARG:HB2	1.94	0.49
1:B:324:ILE:O	1:B:328:MSE:N	2.45	0.49
1:B:325:LYS:O	1:B:329:GLU:HB2	2.13	0.49
1:B:281:ARG:NH1	1:B:357:ARG:HE	2.10	0.49
1:B:400:GLU:HG2	1:B:511:LYS:HZ1	1.77	0.49
1:B:228:PRO:HB3	1:B:382:THR:HA	1.95	0.49
1:B:583:GLU:HG3	1:B:587:GLN:HE21	1.77	0.49
1:B:395:ILE:CD1	1:B:542:SER:HA	2.42	0.48
1:A:340:ARG:HG2	1:A:340:ARG:HH11	1.78	0.48
1:A:503:PHE:N	1:A:504:PRO:CD	2.76	0.48
1:A:421:GLN:O	1:A:425:LYS:HG3	2.13	0.48
1:B:536:ASN:O	1:B:540:ARG:HG3	2.14	0.48
1:B:282:SER:O	1:B:283:VAL:HG13	2.13	0.48
1:B:587:GLN:O	1:B:591:ARG:HG3	2.14	0.48
1:B:365:GLY:C	1:B:367:ARG:H	2.15	0.48
1:A:513:ALA:O	1:A:517:VAL:HG23	2.14	0.48
1:A:326:MSE:O	1:A:330:ARG:HG2	2.14	0.47
1:A:311:PRO:HG3	1:A:330:ARG:HB2	1.96	0.47
1:A:283:VAL:HB	1:A:356:PHE:CE2	2.49	0.47
1:A:503:PHE:HE2	1:A:552:MSE:HE1	1.80	0.47
1:B:515:GLU:O	1:B:518:LYS:HB2	2.14	0.47
1:B:357:ARG:HH11	1:B:357:ARG:HG3	1.79	0.47
1:B:289:HIS:O	1:B:292:TRP:HB3	2.15	0.47
1:A:337:ARG:HE	1:A:495:GLU:CD	2.17	0.47
1:B:470:THR:O	1:B:474:ILE:HG13	2.15	0.47
1:B:503:PHE:N	1:B:504:PRO:CD	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:N	1:B:284:ASN:HD22	2.13	0.46
1:B:287:TYR:HA	1:B:290:PHE:HD2	1.80	0.46
1:B:254:VAL:HB	1:B:332:GLN:NE2	2.31	0.46
1:A:467:ALA:O	1:A:470:THR:HB	2.16	0.46
1:B:338:MSE:SE	1:B:344:ILE:HG21	2.66	0.46
1:A:269:TYR:HE2	1:A:286:ARG:HB3	1.81	0.46
1:A:564:ASN:HB2	1:B:460:LEU:HD22	1.98	0.46
1:A:300:LYS:HA	1:A:375:ALA:HB1	1.98	0.46
1:A:300:LYS:HD3	1:A:301:PHE:CE1	2.51	0.46
1:A:577:PHE:CZ	1:A:581:ILE:HD11	2.51	0.46
1:A:501:GLY:O	1:A:504:PRO:HD2	2.15	0.45
1:B:490:MSE:HE2	1:B:490:MSE:HA	1.98	0.45
1:A:285:HIS:ND1	1:A:289:HIS:ND1	2.53	0.45
1:B:345:SER:HA	1:B:350:PHE:HD2	1.78	0.45
1:A:286:ARG:O	1:A:287:TYR:C	2.54	0.45
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.82	0.45
1:A:430:PRO:O	1:A:433:LYS:N	2.50	0.45
1:B:503:PHE:HE2	1:B:552:MSE:HE1	1.82	0.45
1:A:585:LEU:HD13	1:B:574:GLN:HB3	1.98	0.45
1:B:311:PRO:CG	1:B:330:ARG:HB2	2.46	0.45
1:B:574:GLN:O	1:B:577:PHE:HB3	2.16	0.45
1:B:351:GLN:O	1:B:354:LEU:N	2.47	0.45
1:B:219:TYR:CZ	1:B:540:ARG:HB3	2.52	0.45
1:B:228:PRO:HG2	1:B:231:LYS:HG2	1.99	0.45
1:B:473:GLU:OE1	1:B:584:LYS:NZ	2.48	0.45
1:A:518:LYS:C	1:A:520:SER:H	2.20	0.44
1:A:359:GLU:OE1	1:A:359:GLU:HA	2.18	0.44
1:A:358:ASP:OD1	1:A:360:LYS:HB2	2.17	0.44
1:A:229:LYS:N	1:A:229:LYS:HD2	2.32	0.44
1:B:310:LEU:O	1:B:311:PRO:O	2.35	0.44
1:A:571:LEU:HB2	1:B:589:LEU:HD13	2.00	0.44
1:A:538:VAL:O	1:A:541:VAL:HG12	2.17	0.44
1:A:429:GLY:O	1:A:432:PRO:HD2	2.18	0.44
1:B:422:GLU:HA	1:B:425:LYS:CE	2.48	0.44
1:A:436:GLN:O	1:A:440:LYS:HG2	2.18	0.44
1:A:295:GLU:O	1:A:299:VAL:HG23	2.18	0.44
1:A:466:GLU:OE1	1:A:466:GLU:HA	2.18	0.44
1:B:254:VAL:HB	1:B:332:GLN:HE21	1.83	0.44
1:A:522:LYS:HD3	1:A:522:LYS:C	2.39	0.43
1:A:373:GLU:CD	1:A:373:GLU:N	2.72	0.43
1:A:274:LEU:HD11	1:A:290:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ARG:O	1:B:287:TYR:C	2.56	0.43
1:B:416:LEU:HD13	1:B:493:ASN:HD21	1.83	0.43
1:A:430:PRO:HG2	1:A:431:LEU:H	1.84	0.43
1:A:402:VAL:HG12	1:A:507:ILE:HD11	2.00	0.43
1:B:352:GLN:HE21	1:B:352:GLN:CA	2.32	0.43
1:A:253:VAL:O	1:A:274:LEU:HA	2.19	0.43
1:B:489:LEU:HA	1:B:566:VAL:CG2	2.47	0.43
1:A:398:LYS:HE2	1:A:549:GLN:OE1	2.19	0.43
1:A:348:GLU:OE2	1:A:368:LYS:HE3	2.17	0.43
1:A:218:GLN:O	1:A:222:ALA:HB2	2.19	0.43
1:B:357:ARG:HB2	1:B:361:GLU:OE2	2.18	0.43
1:A:558:ASN:N	1:A:558:ASN:HD22	2.16	0.43
1:B:364:THR:HG23	1:B:365:GLY:N	2.34	0.43
1:A:417:LEU:HD23	1:A:490:MSE:SE	2.68	0.43
1:A:426:ARG:HB2	1:A:426:ARG:HH11	1.81	0.42
1:A:379:ILE:HG23	1:A:380:PHE:N	2.34	0.42
1:B:390:LEU:HD12	1:B:545:SER:HB3	2.00	0.42
1:B:305:ILE:HA	1:B:306:PRO:HD3	1.87	0.42
1:A:251:ASP:CG	1:A:252:CYS:H	2.21	0.42
1:A:566:VAL:HG13	1:A:567:ILE:N	2.35	0.42
1:B:326:MSE:HG3	1:B:326:MSE:O	2.19	0.42
1:A:345:SER:HA	1:A:350:PHE:HD2	1.80	0.42
1:B:299:VAL:O	1:B:375:ALA:HB1	2.19	0.42
1:A:311:PRO:CG	1:A:330:ARG:HB2	2.50	0.42
1:B:588:ALA:HA	1:B:591:ARG:HD2	2.01	0.42
1:A:564:ASN:HB2	1:B:460:LEU:HD13	2.02	0.42
1:A:396:GLU:HG3	1:A:514:ILE:HD13	2.01	0.42
1:B:250:PHE:HB2	1:B:278:ASN:HB2	2.00	0.42
1:B:538:VAL:O	1:B:541:VAL:HG12	2.20	0.42
1:A:587:GLN:HA	1:A:587:GLN:HE21	1.85	0.42
1:B:594:VAL:O	1:B:595:MSE:CB	2.68	0.42
1:B:398:LYS:HG2	1:B:549:GLN:NE2	2.35	0.42
1:B:445:LEU:HG	1:B:449:PHE:CZ	2.54	0.42
1:A:390:LEU:HG	1:A:546:TYR:CE1	2.55	0.42
1:A:292:TRP:CZ2	1:A:366:LYS:HA	2.54	0.41
1:B:224:GLN:C	1:B:226:ALA:H	2.21	0.41
1:B:416:LEU:HD13	1:B:493:ASN:ND2	2.35	0.41
1:B:571:LEU:O	1:B:575:VAL:HG23	2.21	0.41
1:A:463:ALA:HB2	1:A:591:ARG:O	2.19	0.41
1:B:461:ASN:N	1:B:461:ASN:HD22	2.19	0.41
1:B:495:GLU:HG2	1:B:499:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:HG2	1:A:379:ILE:HD13	2.02	0.41
1:A:529:ILE:HB	1:A:533:ASP:CB	2.50	0.41
1:B:392:LEU:HD11	1:B:517:VAL:CG1	2.46	0.41
1:B:224:GLN:C	1:B:226:ALA:N	2.73	0.41
1:A:458:THR:O	1:A:462:ASP:HB2	2.20	0.41
1:B:241:PRO:CG	1:B:549:GLN:HB2	2.51	0.41
1:B:241:PRO:O	1:B:550:ALA:HA	2.21	0.41
1:A:392:LEU:HA	1:A:392:LEU:HD12	1.85	0.41
1:B:480:GLU:O	1:B:483:LYS:HG2	2.21	0.41
1:B:443:GLN:HG3	1:B:468:GLY:HA3	2.03	0.41
1:B:254:VAL:O	1:B:255:ALA:HB2	2.21	0.40
1:B:311:PRO:HG3	1:B:330:ARG:CB	2.51	0.40
1:A:586:ARG:HD2	1:A:586:ARG:HH11	1.77	0.40
1:A:379:ILE:HG13	1:A:383:MSE:HE3	2.03	0.40
1:B:351:GLN:O	1:B:352:GLN:C	2.60	0.40
1:A:583:GLU:OE1	1:A:586:ARG:NH1	2.54	0.40
1:A:552:MSE:HG3	1:A:556:HIS:CD2	2.57	0.40
1:A:405:PHE:CE1	1:B:452:SER:HB3	2.56	0.40
1:B:520:SER:OG	1:B:534:LYS:HE2	2.20	0.40
1:A:287:TYR:O	1:A:290:PHE:HB2	2.21	0.40
1:A:298:LEU:O	1:A:302:GLY:HA3	2.22	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	357/392 (91%)	317 (89%)	36 (10%)	4 (1%)	17	62
1	B	362/392 (92%)	323 (89%)	33 (9%)	6 (2%)	11	52
All	All	719/784 (92%)	640 (89%)	69 (10%)	10 (1%)	14	57

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ARG
1	B	311	PRO
1	A	224	GLN
1	B	255	ALA
1	B	323	PHE
1	A	280	ASN
1	B	308	PRO
1	B	314	GLN
1	B	393	VAL
1	A	430	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	323/333 (97%)	296 (92%)	27 (8%)	14	48
1	B	325/333 (98%)	303 (93%)	22 (7%)	20	59
All	All	648/666 (97%)	599 (92%)	49 (8%)	16	55

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	LYS
1	A	227	LYS
1	A	229	LYS
1	A	230	GLU
1	A	235	ILE
1	A	275	THR
1	A	280	ASN
1	A	291	ASP
1	A	309	SER
1	A	355	ASN
1	A	373	GLU
1	A	384	GLU
1	A	391	ASP

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Mol	Chain	Res	Type
1	A	393	VAL
1	A	397	GLN
1	A	398	LYS
1	A	407	LYS
1	A	409	MSE
1	A	426	ARG
1	A	466	GLU
1	A	511	LYS
1	A	522	LYS
1	A	528	LYS
1	A	558	ASN
1	A	587	GLN
1	A	591	ARG
1	A	595	MSE
1	B	218	GLN
1	B	224	GLN
1	B	230	GLU
1	B	239	TYR
1	B	309	SER
1	B	329	GLU
1	B	331	LEU
1	B	351	GLN
1	B	352	GLN
1	B	358	ASP
1	B	373	GLU
1	B	389	ASP
1	B	416	LEU
1	B	426	ARG
1	B	437	LYS
1	B	447	THR
1	B	459	ASP
1	B	504	PRO
1	B	522	LYS
1	B	530	THR
1	B	535	GLN
1	B	595	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
1	A	280	ASN

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Mol	Chain	Res	Type
1	A	332	GLN
1	A	352	GLN
1	A	436	GLN
1	A	455	GLN
1	A	461	ASN
1	A	487	HIS
1	A	493	ASN
1	A	510	HIS
1	A	532	GLN
1	A	535	GLN
1	A	558	ASN
1	A	564	ASN
1	A	587	GLN
1	B	273	GLN
1	B	284	ASN
1	B	332	GLN
1	B	351	GLN
1	B	352	GLN
1	B	397	GLN
1	B	461	ASN
1	B	510	HIS
1	B	535	GLN
1	B	587	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	350/392 (89%)	-0.26	8 (2%) 64 49	30, 54, 87, 100	0
1	B	355/392 (90%)	-0.19	12 (3%) 49 34	33, 59, 92, 99	0
All	All	705/784 (89%)	-0.22	20 (2%) 56 42	30, 56, 88, 100	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	THR	4.9
1	B	317	GLY	3.2
1	A	248	SER	3.2
1	B	314	GLN	2.9
1	B	268	SER	2.7
1	B	315	VAL	2.6
1	A	225	LEU	2.6
1	B	313	LYS	2.6
1	B	269	TYR	2.5
1	B	322	GLU	2.4
1	A	397	GLN	2.3
1	A	256	ASP	2.3
1	B	224	GLN	2.2
1	B	455	GLN	2.2
1	A	247	THR	2.2
1	B	225	LEU	2.1
1	A	322	GLU	2.1
1	B	226	ALA	2.1
1	A	321	GLU	2.1
1	A	269	TYR	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 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.