



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:01 PM UTC

PDB ID : 2QX5 / pdb_00002qx5
Title : Structure of nucleoporin Nic96
Authors : Jeudy, S.; Schwartz, T.U.
Deposited on : 2007-08-10
Resolution : 2.50 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

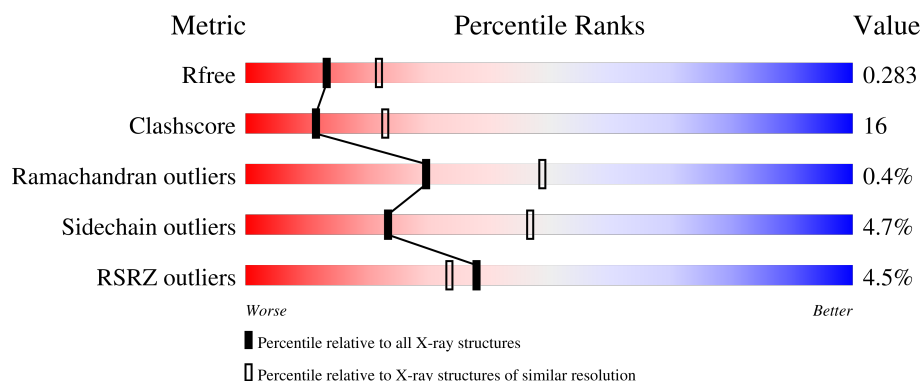
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	661	3% 61% 22% • 14%
1	B	661	4% 60% 23% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9160 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 Nucleoporin NIC96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4521	2910	752	842	17			
1	B	569	Total	C	N	O	S	0	0	0
			4514	2896	754	847	17			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	PRO	-	expression tag	UNP P34077
A	180	GLY	-	expression tag	UNP P34077
A	181	SER	-	expression tag	UNP P34077
A	182	GLU	-	expression tag	UNP P34077
A	183	PHE	-	expression tag	UNP P34077
A	184	GLU	-	expression tag	UNP P34077
A	185	LEU	-	expression tag	UNP P34077
B	179	PRO	-	expression tag	UNP P34077
B	180	GLY	-	expression tag	UNP P34077
B	181	SER	-	expression tag	UNP P34077
B	182	GLU	-	expression tag	UNP P34077
B	183	PHE	-	expression tag	UNP P34077
B	184	GLU	-	expression tag	UNP P34077
B	185	LEU	-	expression tag	UNP P34077

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

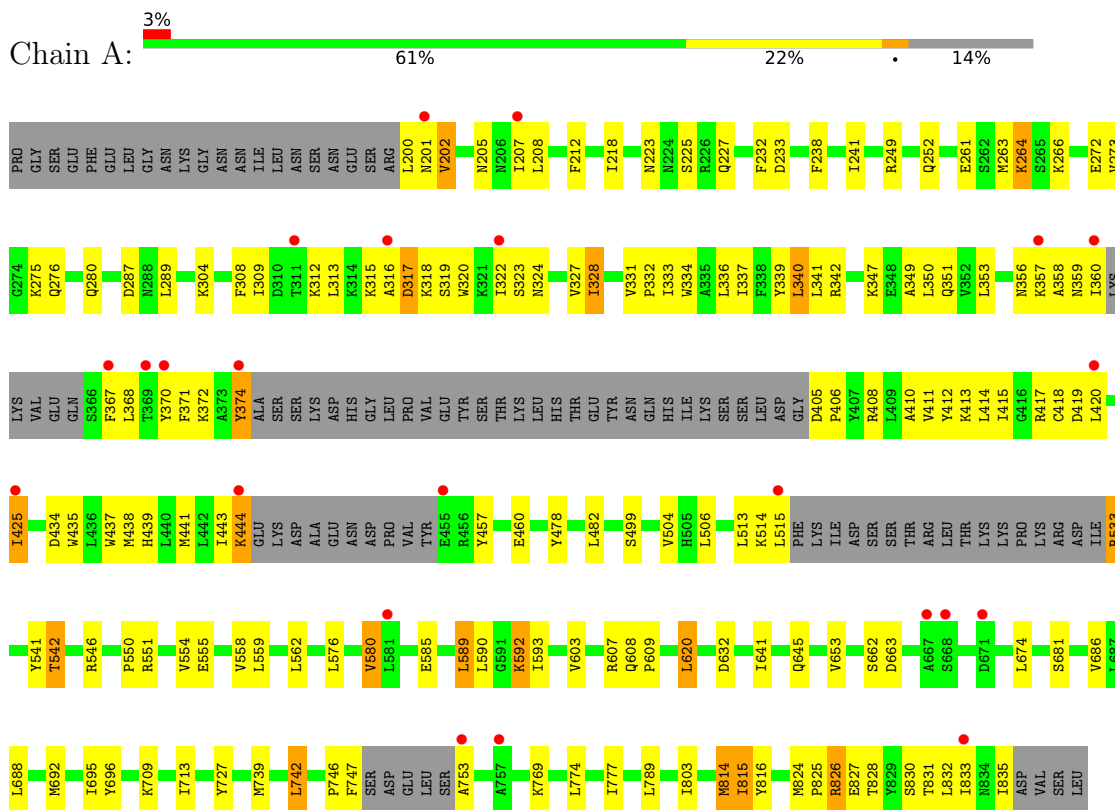
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	60	Total 60	O 60	0	0

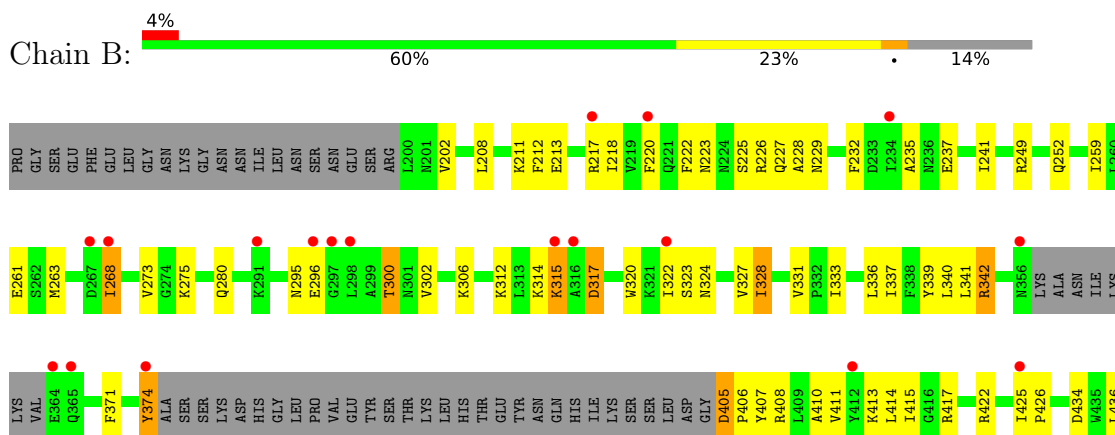
3 Residue-property plots

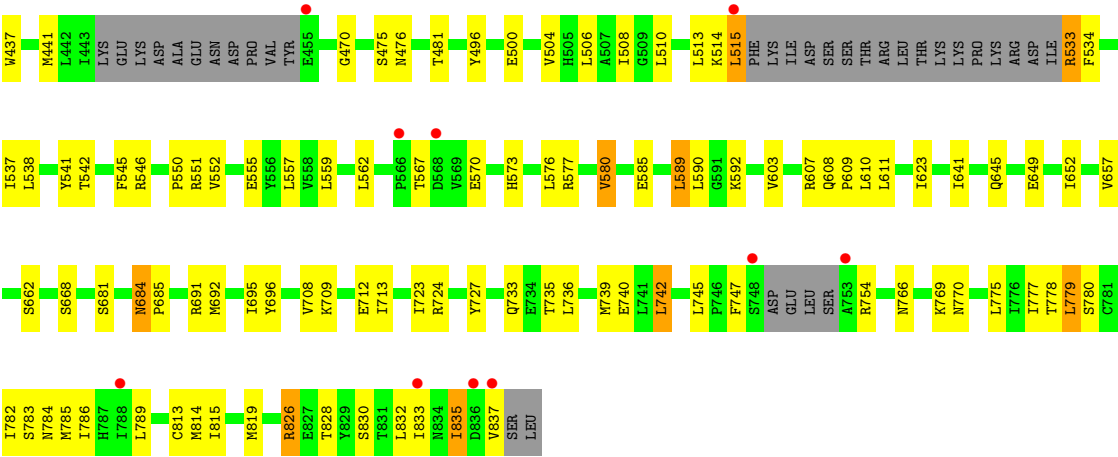
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoporin NIC96



- Molecule 1: Nucleoporin NIC96





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.12Å 82.48Å 113.03Å 90.00° 91.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.50) 99.0 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.41 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.285 0.232 , 0.283	Depositor DCC
R_{free} test set	3118 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9160	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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 52.13 % 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 5.0839e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.46	0/4597	0.83	5/6227 (0.1%)
1	B	0.45	0/4590	0.81	4/6222 (0.1%)
All	All	0.46	0/9187	0.82	9/12449 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	425	ILE	CA-C-N	8.22	128.17	119.05
1	A	425	ILE	C-N-CA	8.22	128.17	119.05
1	A	331	VAL	CA-C-N	6.59	128.08	119.84
1	A	331	VAL	C-N-CA	6.59	128.08	119.84
1	B	470	GLY	CA-C-N	6.48	126.41	119.28
1	B	470	GLY	C-N-CA	6.48	126.41	119.28
1	A	824	MET	N-CA-C	-6.40	102.46	108.22
1	B	684	ASN	CA-C-N	5.83	125.69	119.28
1	B	684	ASN	C-N-CA	5.83	125.69	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	315	LYS	Peptide

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	4521	0	4530	141	0
1	B	4514	0	4486	147	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	63	0	0	2	0
3	B	60	0	0	5	0
All	All	9160	0	9016	288	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 16.

All (288) 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:533:ARG:HH11	1:B:533:ARG:HB2	1.07	1.15
1:A:357:LYS:O	1:A:360:ILE:HG12	1.46	1.12
1:A:533:ARG:HH11	1:A:533:ARG:HB2	0.96	1.11
1:B:533:ARG:HH11	1:B:533:ARG:CB	1.64	1.10
1:A:533:ARG:HB2	1:A:533:ARG:NH1	1.72	1.03
1:B:405:ASP:OD1	1:B:406:PRO:HD2	1.62	0.99
1:B:740:GLU:HG2	1:B:747:PHE:CE2	1.99	0.97
1:B:220:PHE:HD1	1:B:555:GLU:HG2	1.31	0.96
1:B:374:TYR:HD2	1:B:374:TYR:C	1.74	0.95
1:A:826:ARG:HG3	1:A:826:ARG:HH11	1.30	0.95
1:A:533:ARG:HH11	1:A:533:ARG:CB	1.81	0.93
1:B:533:ARG:HB2	1:B:533:ARG:NH1	1.83	0.93
1:B:220:PHE:CD1	1:B:555:GLU:HG2	2.05	0.92
1:A:374:TYR:HD2	1:A:374:TYR:C	1.79	0.91
1:B:649:GLU:HG2	1:B:652:ILE:HD12	1.53	0.89
1:B:826:ARG:HG3	1:B:826:ARG:HH11	1.38	0.86
1:A:825:PRO:HG2	1:A:828:THR:HG23	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:TYR:C	1:B:374:TYR:CD2	2.45	0.86
1:A:341:LEU:HD11	1:A:415:ILE:HD11	1.58	0.85
1:B:733:GLN:HG3	3:B:871:HOH:O	1.76	0.85
1:A:374:TYR:C	1:A:374:TYR:CD2	2.50	0.85
1:B:218:ILE:HD11	1:B:241:ILE:HD12	1.62	0.81
1:A:554:VAL:HG11	1:A:603:VAL:HG12	1.63	0.81
1:B:740:GLU:HG2	1:B:747:PHE:CD2	2.16	0.80
1:B:736:LEU:O	1:B:740:GLU:HG3	1.82	0.80
1:A:309:ILE:HG23	1:A:313:LEU:HD12	1.65	0.78
1:B:814:MET:HA	1:B:814:MET:HE2	1.65	0.78
1:A:645:GLN:CD	1:A:692:MET:HE1	2.10	0.77
1:B:649:GLU:CG	1:B:652:ILE:HD12	2.14	0.77
1:B:786:ILE:HD12	1:B:837:VAL:HG22	1.67	0.76
1:B:405:ASP:OD1	1:B:406:PRO:CD	2.34	0.76
1:B:551:ARG:HG2	1:B:603:VAL:HG21	1.67	0.76
1:B:709:LYS:HE3	1:B:713:ILE:HD11	1.68	0.76
1:B:782:ILE:HG22	1:B:837:VAL:HG21	1.67	0.75
1:B:533:ARG:HH11	1:B:533:ARG:CG	1.97	0.75
1:B:249:ARG:HH11	1:B:252:GLN:HE22	1.37	0.73
1:A:653:VAL:CG1	1:A:692:MET:HE3	2.17	0.73
1:A:353:LEU:HD23	1:A:368:LEU:HD13	1.71	0.73
1:B:573:HIS:O	1:B:577:ARG:HG3	1.88	0.73
1:A:264:LYS:HG2	1:A:513:LEU:HD21	1.71	0.72
1:B:405:ASP:OD1	1:B:405:ASP:C	2.34	0.71
1:A:357:LYS:O	1:A:360:ILE:CG1	2.34	0.71
1:A:826:ARG:HH11	1:A:826:ARG:CG	2.02	0.71
1:A:825:PRO:HG2	1:A:828:THR:CG2	2.21	0.70
1:A:405:ASP:HB2	1:A:406:PRO:HD2	1.72	0.70
1:A:218:ILE:HD11	1:A:241:ILE:HD12	1.72	0.70
1:A:662:SER:OG	1:A:769:LYS:HE2	1.93	0.69
1:A:641:ILE:O	1:A:645:GLN:HG3	1.92	0.69
1:A:275:LYS:HG2	1:A:441:MET:HE2	1.75	0.68
1:B:405:ASP:O	1:B:408:ARG:N	2.26	0.68
1:A:434:ASP:O	1:A:438:MET:HG2	1.93	0.68
1:B:437:TRP:CZ2	1:B:441:MET:HE3	2.29	0.67
1:A:370:TYR:CE2	1:A:415:ILE:HG22	2.29	0.67
1:B:826:ARG:HH11	1:B:826:ARG:CG	2.07	0.66
1:A:815:ILE:HG13	1:A:816:TYR:N	2.09	0.66
1:B:641:ILE:O	1:B:645:GLN:HG3	1.96	0.66
1:A:827:GLU:O	1:A:831:THR:HG23	1.96	0.65
1:B:227:GLN:NE2	1:B:607:ARG:HH11	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:MET:HE1	1:B:832:LEU:HD21	1.77	0.65
1:A:333:ILE:O	1:A:337:ILE:HG13	1.97	0.64
1:A:653:VAL:HG11	1:A:692:MET:HE3	1.79	0.64
1:A:334:TRP:CE2	1:A:408:ARG:HG3	2.32	0.64
1:A:515:LEU:HD12	1:A:515:LEU:O	1.97	0.64
1:A:317:ASP:HB2	1:A:319:SER:OG	1.98	0.64
1:B:783:SER:HA	1:B:837:VAL:HG23	1.79	0.64
1:B:786:ILE:HD12	1:B:837:VAL:CG2	2.28	0.62
1:A:443:ILE:HG22	1:A:444:LYS:HG2	1.79	0.62
1:A:559:LEU:O	1:A:562:LEU:HB2	1.99	0.62
1:B:300:THR:HG22	1:B:302:VAL:N	2.14	0.62
1:A:439:HIS:HD2	1:A:457:TYR:OH	1.82	0.62
1:B:814:MET:HE2	1:B:814:MET:CA	2.30	0.62
1:A:320:TRP:CH2	1:A:332:PRO:HD3	2.34	0.62
1:A:832:LEU:O	1:A:835:ILE:HG22	2.00	0.61
1:B:533:ARG:NH1	1:B:533:ARG:CG	2.60	0.61
1:B:754:ARG:HG2	1:B:819:MET:HE1	1.81	0.61
1:B:830:SER:O	1:B:833:ILE:HG22	2.00	0.61
1:A:342:ARG:NH1	1:A:434:ASP:OD1	2.33	0.61
1:B:496:TYR:CE2	1:B:500:GLU:HG3	2.36	0.61
1:B:410:ALA:O	1:B:414:LEU:HG	2.01	0.61
1:B:315:LYS:O	1:B:317:ASP:N	2.30	0.60
1:A:264:LYS:HB2	1:A:264:LYS:NZ	2.17	0.60
1:B:317:ASP:N	1:B:317:ASP:OD1	2.33	0.60
1:A:350:LEU:HD11	1:A:372:LYS:HG2	1.84	0.60
1:A:315:LYS:O	1:A:316:ALA:HB3	2.02	0.59
1:B:405:ASP:O	1:B:407:TYR:N	2.36	0.59
1:B:550:PRO:HG2	1:B:585:GLU:HG3	1.84	0.58
1:B:227:GLN:HE22	1:B:607:ARG:HD3	1.68	0.58
1:A:413:LYS:NZ	1:A:419:ASP:HB3	2.17	0.58
1:A:592:LYS:NZ	1:A:592:LYS:HB3	2.18	0.58
1:B:275:LYS:HD2	3:B:864:HOH:O	2.03	0.58
1:A:410:ALA:O	1:A:414:LEU:HG	2.04	0.58
1:A:309:ILE:HD11	1:A:336:LEU:HA	1.85	0.58
1:B:567:THR:O	1:B:570:GLU:HG2	2.04	0.58
1:A:327:VAL:C	1:A:328:ILE:HD12	2.28	0.57
1:A:709:LYS:HE3	1:A:713:ILE:HD11	1.86	0.57
1:B:220:PHE:HZ	1:B:552:VAL:HG22	1.69	0.57
1:A:826:ARG:HG3	1:A:826:ARG:NH1	2.12	0.57
1:B:708:VAL:O	1:B:712:GLU:HG3	2.04	0.57
1:A:249:ARG:HH11	1:A:252:GLN:HE22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:MET:HE1	1:A:832:LEU:HD23	1.87	0.56
1:B:218:ILE:HD11	1:B:241:ILE:CD1	2.34	0.56
1:B:542:THR:O	1:B:546:ARG:HG3	2.04	0.56
1:B:223:ASN:HD22	1:B:555:GLU:HG3	1.71	0.56
1:A:405:ASP:CB	1:A:406:PRO:HD2	2.35	0.56
1:A:709:LYS:O	1:A:713:ILE:HG12	2.06	0.56
1:A:202:VAL:HG11	1:A:212:PHE:CG	2.41	0.56
1:A:287:ASP:OD1	1:A:304:LYS:HD3	2.06	0.56
1:B:249:ARG:HH11	1:B:252:GLN:NE2	2.02	0.55
1:A:233:ASP:OD1	1:A:264:LYS:HE2	2.06	0.55
1:B:709:LYS:O	1:B:713:ILE:HG12	2.07	0.55
1:A:695:ILE:HG22	1:A:696:TYR:CD1	2.42	0.55
1:B:814:MET:HA	1:B:814:MET:CE	2.37	0.55
1:A:323:SER:O	1:A:324:ASN:HB2	2.07	0.54
1:A:746:PRO:HB3	1:A:753:ALA:HA	1.89	0.54
1:A:358:ALA:C	1:A:360:ILE:H	2.15	0.54
1:B:333:ILE:O	1:B:337:ILE:HG13	2.07	0.54
1:A:420:LEU:HD12	1:A:420:LEU:H	1.73	0.54
1:B:723:ILE:HG23	1:B:735:THR:HG23	1.89	0.53
1:B:815:ILE:HG22	1:B:819:MET:HE2	1.89	0.53
1:A:316:ALA:C	1:A:318:LYS:H	2.16	0.53
1:B:249:ARG:NH1	1:B:252:GLN:HE22	2.04	0.53
1:B:342:ARG:NH1	1:B:434:ASP:OD1	2.41	0.53
1:B:223:ASN:HA	1:B:226:ARG:HD3	1.90	0.53
1:B:263:MET:HE2	1:B:273:VAL:HG11	1.89	0.53
1:B:510:LEU:O	1:B:515:LEU:HB2	2.08	0.53
1:A:308:PHE:CE1	1:A:312:LYS:HG3	2.44	0.53
1:B:302:VAL:CG1	1:B:306:LYS:HE3	2.39	0.53
1:B:496:TYR:HE2	1:B:500:GLU:HG3	1.74	0.52
1:A:405:ASP:OD1	1:A:405:ASP:C	2.53	0.52
1:A:504:VAL:HG21	1:A:541:TYR:HB2	1.91	0.52
1:A:830:SER:O	1:A:833:ILE:HG22	2.09	0.52
1:A:370:TYR:HE2	1:A:415:ILE:HG22	1.73	0.52
1:A:367:PHE:HB2	1:A:412:TYR:CZ	2.45	0.52
1:B:782:ILE:HG22	1:B:837:VAL:CG2	2.38	0.52
1:A:227:GLN:NE2	1:A:607:ARG:HH11	2.08	0.51
1:A:261:GLU:HA	1:A:264:LYS:HE3	1.90	0.51
1:A:832:LEU:HD23	1:A:832:LEU:C	2.36	0.51
1:B:542:THR:HA	1:B:545:PHE:CE2	2.46	0.51
1:A:413:LYS:HD2	1:A:425:ILE:HD13	1.91	0.51
1:B:514:LYS:O	1:B:515:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD23	1:A:349:ALA:HA	1.93	0.50
1:A:327:VAL:O	1:A:328:ILE:HD12	2.11	0.50
1:B:577:ARG:NH2	1:B:623:ILE:HA	2.25	0.50
1:A:835:ILE:HG23	1:A:835:ILE:O	2.10	0.50
1:A:309:ILE:CD1	1:A:336:LEU:HA	2.41	0.50
1:B:300:THR:HG22	1:B:302:VAL:H	1.76	0.50
1:B:542:THR:HA	1:B:545:PHE:CZ	2.46	0.50
1:B:739:MET:O	1:B:742:LEU:HB2	2.11	0.50
1:B:322:ILE:HD11	1:B:407:TYR:HE1	1.76	0.50
1:B:695:ILE:HG22	1:B:696:TYR:CD1	2.47	0.50
1:A:232:PHE:HE1	3:A:903:HOH:O	1.94	0.50
1:B:692:MET:HA	1:B:692:MET:HE2	1.94	0.49
1:B:295:ASN:O	1:B:296:GLU:C	2.55	0.49
1:B:580:VAL:HG12	1:B:589:LEU:HD23	1.94	0.49
1:A:347:LYS:O	1:A:351:GLN:HG3	2.13	0.49
1:A:592:LYS:HG2	1:A:593:ILE:N	2.27	0.49
1:B:826:ARG:CG	1:B:826:ARG:NH1	2.72	0.49
1:A:645:GLN:CG	1:A:692:MET:HE1	2.42	0.49
1:A:322:ILE:HD11	1:A:406:PRO:HG3	1.94	0.49
1:B:302:VAL:HG12	1:B:306:LYS:HE3	1.93	0.49
1:B:662:SER:OG	1:B:769:LYS:HE2	2.12	0.49
1:A:425:ILE:HD11	1:A:438:MET:HE1	1.93	0.49
1:A:200:LEU:CD1	1:A:208:LEU:HD21	2.43	0.49
1:B:323:SER:O	1:B:324:ASN:HB2	2.13	0.48
1:B:336:LEU:O	1:B:340:LEU:HG	2.12	0.48
1:A:353:LEU:HD22	1:A:371:PHE:HD2	1.77	0.48
1:A:478:TYR:CE2	1:A:482:LEU:HD11	2.47	0.48
1:A:789:LEU:HB2	1:A:803:ILE:HD11	1.95	0.48
1:A:592:LYS:HB3	1:A:592:LYS:HZ3	1.79	0.48
1:A:550:PRO:CG	1:A:585:GLU:HG3	2.44	0.48
1:A:443:ILE:CG2	1:A:444:LYS:N	2.76	0.47
1:A:739:MET:O	1:A:742:LEU:HB2	2.14	0.47
1:A:576:LEU:O	1:A:580:VAL:HG13	2.14	0.47
1:B:213:GLU:O	1:B:217:ARG:HG3	2.13	0.47
1:B:324:ASN:O	1:B:405:ASP:HB2	2.15	0.47
1:B:328:ILE:O	1:B:331:VAL:HG12	2.14	0.47
1:B:832:LEU:C	1:B:832:LEU:HD23	2.40	0.47
1:A:674:LEU:HD13	1:A:686:VAL:HG21	1.97	0.47
1:A:356:ASN:O	1:A:357:LYS:C	2.58	0.47
1:A:368:LEU:HD12	1:A:368:LEU:O	2.15	0.47
1:A:417:ARG:O	1:A:420:LEU:HD11	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:TYR:CD1	1:A:777:ILE:HG23	2.50	0.47
1:B:259:ILE:O	1:B:263:MET:HE3	2.14	0.47
1:B:657:VAL:HG21	1:B:692:MET:HG3	1.95	0.47
1:B:745:LEU:HD13	1:B:775:LEU:HD23	1.95	0.47
1:B:405:ASP:O	1:B:406:PRO:C	2.58	0.47
1:B:832:LEU:HD23	1:B:832:LEU:O	2.15	0.46
1:B:835:ILE:HG23	1:B:835:ILE:O	2.15	0.46
1:A:249:ARG:HH11	1:A:252:GLN:NE2	2.13	0.46
1:B:314:LYS:HE3	1:B:320:TRP:CH2	2.50	0.46
1:B:322:ILE:HG13	1:B:322:ILE:O	2.16	0.46
1:B:783:SER:HA	1:B:837:VAL:CG2	2.46	0.46
1:B:227:GLN:NE2	1:B:607:ARG:CD	2.79	0.46
1:A:315:LYS:O	1:A:316:ALA:CB	2.62	0.46
1:A:826:ARG:CG	1:A:826:ARG:NH1	2.68	0.46
1:B:533:ARG:O	1:B:537:ILE:HG13	2.15	0.46
1:B:263:MET:HE2	1:B:273:VAL:CG1	2.46	0.45
1:A:340:LEU:HB3	1:A:349:ALA:HB2	1.98	0.45
1:A:826:ARG:HD2	1:A:826:ARG:HA	1.81	0.45
1:A:411:VAL:O	1:A:415:ILE:HG12	2.16	0.45
1:B:727:TYR:CD1	1:B:777:ILE:HG23	2.50	0.45
1:B:268:ILE:O	1:B:268:ILE:HG13	2.16	0.45
1:A:322:ILE:CD1	1:A:406:PRO:HG3	2.46	0.45
1:B:327:VAL:C	1:B:328:ILE:HD12	2.42	0.45
1:B:436:LEU:HD21	1:B:481:THR:HG23	1.97	0.45
1:B:437:TRP:CE2	1:B:441:MET:HE3	2.52	0.45
1:B:223:ASN:OD1	1:B:226:ARG:NH1	2.50	0.45
1:A:832:LEU:O	1:A:835:ILE:CG2	2.63	0.45
1:A:223:ASN:HD22	1:A:555:GLU:HG3	1.82	0.45
1:B:417:ARG:HD2	3:B:894:HOH:O	2.17	0.45
1:A:554:VAL:O	1:A:558:VAL:HG23	2.15	0.44
1:A:444:LYS:N	1:A:457:TYR:O	2.48	0.44
1:A:550:PRO:HG2	1:A:585:GLU:HG3	2.00	0.44
1:B:225:SER:CB	1:B:232:PHE:HB2	2.48	0.44
1:A:620:LEU:HD23	1:A:620:LEU:HA	1.80	0.44
1:B:475:SER:HB3	1:B:476:ASN:H	1.56	0.44
1:B:513:LEU:O	1:B:514:LYS:HB2	2.18	0.44
1:A:663:ASP:OD1	1:A:769:LYS:HE3	2.18	0.44
1:A:263:MET:HE3	1:A:263:MET:HB2	1.89	0.44
1:A:342:ARG:HD2	1:A:437:TRP:CE3	2.53	0.44
1:A:515:LEU:O	1:A:515:LEU:CD1	2.65	0.44
1:B:228:ALA:O	1:B:229:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:O	1:A:276:GLN:HG3	2.18	0.43
1:B:814:MET:HE2	1:B:814:MET:N	2.32	0.43
1:A:312:LYS:O	1:A:313:LEU:HD23	2.19	0.43
1:B:740:GLU:HG2	1:B:747:PHE:CZ	2.50	0.43
1:A:580:VAL:HG12	1:A:589:LEU:HD23	2.00	0.43
1:A:218:ILE:HG21	1:A:238:PHE:CE1	2.53	0.43
1:A:266:LYS:HD2	1:A:273:VAL:HG22	2.01	0.43
1:B:212:PHE:CZ	1:B:552:VAL:HG11	2.54	0.43
1:B:684:ASN:HA	1:B:685:PRO:HD3	1.74	0.43
1:A:747:PHE:N	1:A:747:PHE:CD1	2.87	0.42
1:B:211:LYS:HE3	3:B:846:HOH:O	2.18	0.42
1:A:562:LEU:HD12	1:A:562:LEU:HA	1.73	0.42
1:B:504:VAL:HG21	1:B:541:TYR:HB2	2.00	0.42
1:B:413:LYS:NZ	1:B:422:ARG:O	2.42	0.42
1:B:557:LEU:HA	1:B:557:LEU:HD23	1.78	0.42
1:A:608:GLN:N	1:A:609:PRO:HD2	2.34	0.42
1:B:235:ALA:HB1	1:B:261:GLU:HB2	2.00	0.42
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.95	0.42
1:A:417:ARG:HE	1:A:417:ARG:HB2	1.66	0.42
1:B:295:ASN:O	1:B:295:ASN:CG	2.63	0.42
1:B:668:SER:OG	1:B:724:ARG:NH2	2.48	0.42
1:A:435:TRP:CE2	1:A:439:HIS:CE1	3.08	0.42
1:A:551:ARG:HG2	1:A:603:VAL:HG21	2.02	0.42
1:A:608:GLN:N	1:A:609:PRO:CD	2.82	0.42
1:B:508:ILE:HG12	1:B:559:LEU:HD13	2.00	0.42
1:B:577:ARG:CZ	1:B:623:ILE:HD13	2.50	0.42
1:B:411:VAL:HG13	1:B:415:ILE:HD13	2.02	0.42
1:B:681:SER:HB3	1:B:691:ARG:HD2	2.01	0.42
1:A:339:TYR:HA	1:A:342:ARG:HB3	2.02	0.42
1:A:542:THR:HG22	1:A:546:ARG:HD2	2.00	0.42
1:B:339:TYR:HA	1:B:342:ARG:HB3	2.01	0.42
1:B:785:MET:O	1:B:789:LEU:HG	2.19	0.42
1:A:460:GLU:CD	1:A:460:GLU:H	2.27	0.41
1:B:551:ARG:HD3	3:B:884:HOH:O	2.20	0.41
1:B:576:LEU:HD11	1:B:611:LEU:HD21	2.02	0.41
1:B:371:PHE:CD1	1:B:415:ILE:HG12	2.55	0.41
1:B:580:VAL:HA	1:B:589:LEU:HD23	2.02	0.41
1:B:766:ASN:O	1:B:770:ASN:ND2	2.53	0.41
1:A:340:LEU:HD23	1:A:349:ALA:N	2.34	0.41
1:A:632:ASP:CB	3:A:909:HOH:O	2.68	0.41
1:B:534:PHE:CZ	1:B:538:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:CB	1:A:232:PHE:HB2	2.50	0.41
1:A:227:GLN:HE22	1:A:607:ARG:HD3	1.85	0.41
1:A:420:LEU:HD12	1:A:420:LEU:N	2.35	0.41
1:A:774:LEU:HD23	1:A:774:LEU:HA	1.87	0.41
1:B:775:LEU:O	1:B:779:LEU:HB2	2.20	0.41
1:A:205:ASN:OD1	1:A:207:ILE:HB	2.20	0.41
1:A:358:ALA:C	1:A:360:ILE:N	2.77	0.41
1:B:232:PHE:CZ	1:B:237:GLU:HG3	2.55	0.41
1:B:786:ILE:CD1	1:B:837:VAL:HG22	2.45	0.41
1:A:261:GLU:C	1:A:263:MET:H	2.27	0.41
1:B:220:PHE:CZ	1:B:552:VAL:HG22	2.52	0.41
1:B:739:MET:HG2	1:B:778:THR:OG1	2.20	0.41
1:A:356:ASN:O	1:A:358:ALA:N	2.55	0.40
1:B:607:ARG:HD2	1:B:610:LEU:HD12	2.02	0.40
1:A:513:LEU:O	1:A:514:LYS:HB2	2.20	0.40
1:B:227:GLN:HG3	1:B:610:LEU:HG	2.04	0.40
1:B:322:ILE:HD11	1:B:407:TYR:CE1	2.53	0.40
1:B:608:GLN:N	1:B:609:PRO:HD2	2.36	0.40
1:B:780:SER:O	1:B:784:ASN:ND2	2.54	0.40
1:B:222:PHE:O	1:B:226:ARG:HG3	2.20	0.40
1:B:813:CYS:C	1:B:814:MET:HE2	2.46	0.40
1:A:340:LEU:HD23	1:A:349:ALA:CA	2.51	0.40
1:B:425:ILE:HA	1:B:426:PRO:HD3	1.84	0.40
1:A:357:LYS:O	1:A:360:ILE:CG2	2.68	0.40
1:A:742:LEU:HD12	1:A:742:LEU:HA	1.92	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	557/661 (84%)	537 (96%)	17 (3%)	3 (0%)	24 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	557/661 (84%)	533 (96%)	22 (4%)	2 (0%)	30	49
All	All	1114/1322 (84%)	1070 (96%)	39 (4%)	5 (0%)	30	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	835	ILE
1	A	317	ASP
1	A	499	SER
1	B	268	ILE
1	A	359	ASN

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	490/598 (82%)	466 (95%)	24 (5%)	22	45
1	B	489/598 (82%)	467 (96%)	22 (4%)	24	49
All	All	979/1196 (82%)	933 (95%)	46 (5%)	23	47

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ASN
1	A	202	VAL
1	A	264	LYS
1	A	280	GLN
1	A	289	LEU
1	A	328	ILE
1	A	340	LEU
1	A	374	TYR
1	A	418	CYS
1	A	444	LYS
1	A	506	LEU

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Mol	Chain	Res	Type
1	A	533	ARG
1	A	542	THR
1	A	580	VAL
1	A	589	LEU
1	A	590	LEU
1	A	592	LYS
1	A	620	LEU
1	A	681	SER
1	A	688	LEU
1	A	742	LEU
1	A	814	MET
1	A	815	ILE
1	A	826	ARG
1	B	202	VAL
1	B	208	LEU
1	B	280	GLN
1	B	300	THR
1	B	312	LYS
1	B	317	ASP
1	B	328	ILE
1	B	341	LEU
1	B	342	ARG
1	B	374	TYR
1	B	405	ASP
1	B	506	LEU
1	B	515	LEU
1	B	533	ARG
1	B	580	VAL
1	B	589	LEU
1	B	590	LEU
1	B	592	LYS
1	B	742	LEU
1	B	779	LEU
1	B	826	ARG
1	B	828	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	227	GLN
1	A	246	ASN

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Mol	Chain	Res	Type
1	A	252	GLN
1	A	280	GLN
1	A	329	ASN
1	A	439	HIS
1	A	645	GLN
1	A	707	HIS
1	A	710	ASN
1	A	766	ASN
1	A	770	ASN
1	A	812	GLN
1	A	834	ASN
1	B	206	ASN
1	B	227	GLN
1	B	229	ASN
1	B	252	GLN
1	B	295	ASN
1	B	324	ASN
1	B	329	ASN
1	B	439	HIS
1	B	612	HIS
1	B	707	HIS
1	B	738	GLN
1	B	770	ASN
1	B	773	ASN
1	B	821	GLN
1	B	834	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	569/661 (86%)	0.31	23 (4%) 42 38	31, 56, 100, 135	0
1	B	569/661 (86%)	0.35	28 (4%) 35 31	33, 58, 106, 143	0
All	All	1138/1322 (86%)	0.33	51 (4%) 38 33	31, 58, 102, 143	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	ILE	5.3
1	B	455	GLU	4.2
1	B	568	ASP	3.9
1	B	753	ALA	3.8
1	B	515	LEU	3.7
1	B	364	GLU	3.6
1	B	837	VAL	3.4
1	A	455	GLU	3.3
1	B	220	PHE	3.3
1	A	581	LEU	3.2
1	A	444	LYS	3.2
1	B	356	ASN	3.1
1	A	322	ILE	3.1
1	B	833	ILE	3.0
1	B	268	ILE	2.9
1	B	316	ALA	2.9
1	B	234	ILE	2.9
1	A	667	ALA	2.9
1	A	515	LEU	2.9
1	B	267	ASP	2.8
1	A	367	PHE	2.8
1	B	296	GLU	2.7
1	A	369	THR	2.7
1	B	365	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	374	TYR	2.6
1	A	357	LYS	2.6
1	A	420	LEU	2.5
1	B	315	LYS	2.5
1	B	297	GLY	2.5
1	A	201	ASN	2.5
1	B	748	SER	2.5
1	B	412	TYR	2.5
1	A	757	ALA	2.4
1	A	374	TYR	2.4
1	A	311	THR	2.4
1	A	370	TYR	2.4
1	B	425	ILE	2.3
1	B	788	ILE	2.3
1	A	753	ALA	2.2
1	B	322	ILE	2.2
1	B	836	ASP	2.2
1	B	217	ARG	2.2
1	B	291	LYS	2.1
1	A	207	ILE	2.1
1	A	668	SER	2.1
1	B	298	LEU	2.1
1	A	833	ILE	2.1
1	B	566	PRO	2.0
1	A	316	ALA	2.0
1	A	425	ILE	2.0
1	A	671	ASP	2.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	854	1/1	0.90	0.12	58,58,58,58	0
2	CL	B	844	1/1	0.94	0.08	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.